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6	TEMPERATURE DEPENDENCE OF GAS PROPERTIES IN POLYNOMIAL FORM
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electronic calculators. Using the polynomial approximations and a suitable calculator, it is possible to duplicate existing reference source tabular values directly, obviating the need for interpolation or further reference to the tables per se. The accuracy of the calculated values can be within 0.5% of the tabular values. The polynomial coefficients are given in the International System of Units (SI). Methods are presented to calculate the temperature corresponding to a given property value. Extrapolation features of the polynomials are discussed.

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ABSTRACT

Based on a least-squares polynomial approximation, a procedure is introduced for calculating existing tabular values of thermodynamic and transport properties for common gases. The specific heat at constant pressure is given for 238 gases, the thermal conductivity for 55 gases, the dynamic viscosity for 58 gases, and the second and third virial coefficients for 14 gases. At sufficiently low pressures, ideal gas behavior prevails and temperature may be used as the single independent variable. The algorithm for nested multiplication is presented, optimized for hand-held or desktop electronic calculators. Using the polynomial approximations and a suitable calculator, it is possible to duplicate existing reference source tabular values directly, obviating the need for interpolation or further reference to the tables per se. The accuracy of the calculated values can be within 0.5% of the tabular values. The polynomial coefficients are given in the International System of Units (SI). Methods are presented to calculate the temperature corresponding to a given property value. Extrapolation features of the polynomials are discussed.

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I. INTRODUCTION

Many important thermodynamic and transport properties of gaseous elements and compounds can be expressed purely and accurately as functions of temperature. The perfect gas behavior of simple compressible substances is a well documented example¹⁻³. Data tables for such single-variable functions may be approximated with curve-fitting techniques reducing the tabular information to polynomial or exponential forms. Given these equations and a handheld or desktop electronic calculator, a user may retrieve the tabular information accurately and conveniently without interpolation or further reference to the original data sources. The objective of this work is to provide sufficiently simple polynomial fits which together with a modern electronic calculator present the most convenient method of handling the calculation of thermodynamic properties accurately. In all but the most detailed numerical work, the information presented here should prove to be advantageous over present tabular, graphical, or other methods. This report significantly expands the scope of our earlier work⁴ by including basic properties of a large number of elements and compounds.

The gas properties for which polynomial equations are presented comprise the specific heat at constant pressure [$C_p(T)$] for 238 gases in Appendix A, the thermal conductivity [$k(T)$] for 55 gases in Appendix B, the dynamic viscosity [$\mu(T)$] for 58 gases in Appendix C, and the second and third virial coefficients for 14 gases in Appendix D. The accuracy of reproduction of source data is within 0.5%. The correlating equations are presented in the International System of Units (SI). To further enhance the usefulness of this work, methods are given to reverse the dependent and independent variables (i.e., to calculate the temperature corresponding to a given property

value); these methods consist of either polynomials for the inverse calculation as given in the Appendixes or the iterative procedures discussed in Section 5.

In any effort such as this, consideration must be given to the range of validity of the polynomial fit in addition to its accuracy. Section 2 addresses these important topics. The possibility and limitation of extrapolation is discussed in Section 4. Also, the technique of nested multiplication is discussed in Section 3; this technique is a "natural" for the majority of electronic calculators presently available and provides for the convenient use of the information presented herein.

It should be noted that for a perfect or ideal gas (with variable heat capacities) having C_p in polynomial form is particularly useful. This is because the polynomials may be integrated easily, without risking any decrease in the accuracy of the results. The well known relations for a perfect or ideal gas are summarized below and Ref. 5 expands on the technique for generating the gas tables.

$$C_v = C_p - R \quad [\text{specific heat at constant volume}]$$

$$\gamma = C_p / (C_p - R) \quad [\text{ratio of heat capacities}]$$

$$h = \int C_p dT \quad [\text{enthalphy}]$$

$$u = h - RT \quad [\text{internal energy}]$$

$$\phi = \int C_p \frac{dT}{T} \quad [\text{entropy function}]$$

While the simplicity and utility of the perfect or ideal gas calculations is readily apparent, imperfect or real gas behavior is also important. In the Appendixes, therefore, two headings are often found, i.e., ideal gas and real gas. We also include in this work polynomial fits for the second

and third virial coefficients. These allow accurate representation of non-ideal behavior at densities as high as 0.7 of the critical value⁶.

The material in this report is intended to be used in conjunction with standard reference texts on thermodynamics, fluid dynamics, and heat transfer. The user is encouraged, moreover, to discover for himself how the simple polynomial fits aid in the handling of differential equations with variable coefficients.

II. POLYNOMIAL CURVE FITS

The data source for Appendixes A, B, and C is the TRPC⁷⁻⁹ series. The virial coefficients are found in the American Institute of Physics Handbook, 3rd Edition¹⁰. These sources are considered to be among the most accurate. The TRPC series reproduce a large number of original sources and present a critically evaluated consolidation of available data. The accuracy of duplication of reference-source values is included with the polynomial equations as part of the format in the Appendixes [see pp. A-viii, B-iii, C-iii, and Dii]. References 7-9 include their own third-degree polynomial fits; other polynomial expressions are also available^{11,12} in most thermodynamic textbooks.

The most important consideration given in the curve fitting is the reliability of the data. Next to reliability, consideration is given to the greatest possible temperature range; reference source data are split along temperature intervals to achieve the most acceptable duplication accuracy. The equations presented are the lowest degree equations which achieve the desired accuracy over the temperature range stated.

III. POLYNOMIAL EVALUATIONS

For the calculation of properties or the inverse calculation of the temperature, we have relied almost exclusively on polynomial fits, with the exception of some specific heat [$C_p(T)$] forms which are exponential. The equations presented have the following forms:

Polynomial

$$FCTN(T) = B(0) + B(1)T + B(2)T^2 + \dots + B(N)T^N = \sum_{m=0}^N B(m)T^m$$

Exponential

$$\ln[FCTN(T)] = B(0) + B(1)T + \dots + B(N)T^N = \sum_{m=0}^N B(m)T^m$$

$$[e.g., \quad C_p(T) = (\text{const}) \exp \left[\sum_{m=0}^N B(m)T^m \right]$$

The most efficient method of evaluating single-variable polynomials is "nested multiplication"¹³. Nested multiplication eliminates the need to raise "X" to the "Y" power and simplifies an N-th order polynomial evaluation to a sequence of multiplication/addition steps. Examples of nested multiplication are presented below.

A. Generalized Nested Multiplication Algorithm:

Given the N coefficients, B(0), B(1), B(2), ... B(N), for the polynomial function FCTN(T) and any value of the temperature " T_i " within the range of validity

Set $A(N) = B(N)$ [e.g., $A(6) = B(6)$]

For $K = N, N-1, N-2, \dots, 1$, Do

 Set $A(K-1) = B(K-1) + T_i A(K)$

A(0) = FCTN(T_i)

The above algorithm may be stated in words as follows: multiply the highest degree coefficient by the temperature value, T_i , and add to the next lower degree coefficient; multiply the sum by T_i and add to the next lower degree coefficient; multiply the sum by T_i ... Continue the process until the sum $B(1)+A(2)T_i$ is calculated; multiply this sum by T_i . By just adding the $B(0)$ coefficient to the previous product, the polynomial evaluation is completed for the chosen value of T_i .

B. Specific Example of Nested Multiplication:

Consider the calculation of the specific heat at constant pressure $[C_p(T)]$ for carbon dioxide (CO_2), ideal gas, at $800^{\circ}K$. From page A-9,

$$C_p(T) = 453.86462 + 1.5334795T - 4.195556E-04 T^2 \\ - 1.871946E-06 T^3 + 2.862388E-09 T^4 \\ - 1.6962E-12 T^5 + 3.717285E-16 T^6$$

$$\text{Set } A(6) = 3.717285E-16 ; T = 800$$

Step-by-Step Procedures		Calculated Values		A(N)
(1)	3.717285E-16	B(6)	= 3.717285E-16	A(6)
(2)	X800	XT _i	2.973828E-13	
(3)	-1.6962E-12	+B(5)	-1.3988172E-12	A(5)
(4)	X800	XT _i	-1.11905376E-09	
(5)	+2.862388E-09	+B(4)	1.74333424E-09	A(4)
(6)	X800	XT _i	1.394667392E-06	
(7)	-1.871946E-06	+B(3)	-4.77278608E-07	A(3)
(8)	X800	XT _i	-3.818228864E-04	
(9)	-4.195556E-04	+B(2)	-8.013784864E-04	A(2)
(10)	X800	XT _i	-0.641102789	
(11)	+1.5334795	+B(1)	0.892376711	A(1)
(12)	X800	XT _i	713.9013687	
(13)	+453.86462	+B(0)	1167.765989	A(0)

Rounding to two decimal places, $A(0) = C_p(800K) = 1167.77 \text{ J/Kg K.}$

For programmable calculators, nested multiplication is extremely efficient and highly recommended. To preserve the add-multiply-add simplicity, negative coefficients should be stored as negative values.

IV. EXTRAPOLATION

With each polynomial equation there is a specified range of validity and an associated error estimate. The stated temperature range corresponds to that of the reference source. It is often highly desirable to know how the given polynomial expressions extrapolate. A limited polynomial extrapolation beyond the specified temperature range may often be possible but in indiscriminate extrapolation the accuracy will most likely suffer. In fact, polynomial fits are notoriously bad for certain type of curves outside of their specified range.

Clearly, it is inappropriate to look at every possible type of variation. Suffice it to say that for reasonably smooth, monotonic functions such as the viscosity, the thermal conductivity, and perhaps the heat capacity of polyatomic molecules, the polynomial fits will follow with some fidelity the trends outside of their specified range. If is anticipated that the heat capacity of diatomic molecules will be the most difficult for the polynomials to follow because of the "stepwise" nature of the curves^{14,15}. We have chosen to present the heat capacity of nitrogen as an example. The ideal gas polynomial fits are given on pg. A-41; we choose the curve for the temperature range 590-1365°K. As the basis of comparison, we pick the theoretical¹⁴ curve which represents the activation of the vibrational mode of the nitrogen molecule, using $\theta_v = 3390^\circ\text{K}$. Table I shows a listing of these calculations. It is seen that the polynomial results are within an acceptable $\pm 0.5\%$ for the temperature range 500°K to 1600°K. Above and below this range the polynomial results quickly diverge as more or less anticipated. Certainly, a useful rule may be to stay within 100°K of the guaranteed range.

TABLE I

POLYNOMIAL COMPARISON, C_p FOR NITROGEN

T (K)	CP/R THEO	CP/R POLY	%DIFF
400	3.51513	3.55253	-1.06371
500	3.55272	3.56516	- .35014
600	3.6137	3.62092	- .199842
700	3.68868	3.69739	- .236274
800	3.76795	3.77981	- .314853
900	3.84486	3.85952	- .381236
1000	3.91588	3.9325	- .424339
1100	3.97859	3.99775	- .456325
1200	4.03582	4.05591	- .497772
1300	4.08501	4.10757	- .552173
1400	4.12787	4.15159	- .574591
1500	4.16518	4.18432	- .45953
1600	4.19768	4.19665	.024718
1700	4.22606	4.17417	1.22786
1800	4.2509	4.09448	3.67977

The reader might ask at this point why bother with a polynomial when an exact expression is available. The answer to this question is two-fold: First, reliable analytical expressions are not available for most of the properties and, second, when available they tend to be much more cumbersome than the polynomial expressions presented here.

V. ITERATIVE METHODS

It is often necessary to calculate the temperature from the known value of a property. This inverse problem is handled two ways, either a polynomial fit is given in Appendixes A, B, and C for the calculation of the absolute temperature as a function of the property or an iterative procedure is suggested. In this section we discuss such iterative methods.

Before proceeding, however, it is worth noting that when a second degree polynomials in T is given for the inverse calculation, the quadratic formula may be applied. If it works, this is by far the quickest way to a solution.

The polynomials presented have the absolute temperature (T) as the single independent variable and the property value (PV) as the dependent variable. $FCTN(T_i)$ becomes the magnitude of the property value (PV) when the polynomial function is evaluated at $T = T_i$. Thus, $FCTN(T_i) = |PV|$ at $T = T_i$. To enhance the usefulness of this work, three methods are provided for the calculation of temperature (T) as a function of a known or given property value, PV. The methods are (A) secant method, (B) Newton's method, and (C) fixed point iteration¹⁶. All three methods are iterative in nature.

The general form of the polynomials is

$$FCTN(T_i) = B(0) + B(1)T_i + B(2)T_i^2 + \dots + B(N)T_i^N$$

The iterative methods attempt to solve for the approximate root (the temperature) of the equation of the form

$$F(T_i) = PV - B(0) - B(1)T_i - B(2)T_i^2 - \dots - B(N)T_i^N = 0$$

All of the polynomials are both continuous and continuously differentiable over the temperature intervals specified. Although these conditions are necessary for iterative methods to converge to an approximate root,

they are not necessarily sufficient in all cases to assure convergence. Enough testing has been done with the polynomials presented, however, to give reasonable assurance of convergence with any of the three methods discussed.

The quadratic formula for the second degree polynomial is simply

$$T = \frac{-B(1) + \sqrt{B(1)^2 - 4 B(2)[B(0) - PV]}}{2 B(2)}$$

A. Secant or Interpolation Method^{13,16}:

When it converges, the secant method does so very rapidly, generally more rapidly than either of the other two iterative methods discussed. Two initial values (guesses) for the temperature are required, T_{-1} and T_0 . The initial temperature values selected may be the extremes of the valid temperature range noted with the polynomial sets.

Algorithm: Given $(T_i) = 0$ and two (2) initial points, T_{-1} and T_0

For $n = 0, 1, 2, \dots$ until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - F(T_n) \frac{(T_n - T_{n-1})}{F(T_n) - F(T_{n-1})}$$

In the special case when second degree polynomials given in the Appendix, the secant method algorithm reduces to:

For $n = 0, 1, 2, \dots$ until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - \frac{B(0) + B(1)T_n + B(2)T_n^2 - (PV)}{B(1) + B(2)(T_n + T_{n-1})}$$

Specific Example: Consider a second (2nd) degree polynomial for $C_p(T)$: $FCTN (T_i) = 0.232829 + 1.43429E-05T_i + 3.56638E-09T_i^2$. Assume a given property value $C_p = 0.2567$ but the temperature is unknown. The

known property value (PV) is 0.2567 and T_{-1} and T_0 are chosen arbitrarily at 200 and 2400 respectively. The following solution is provided:

n	T_{n-1}	T_n	T_{n+1}
0	200	2400	-
1	2400	2400	1411.67
2	2400	1411.67	1286.97
3	1411.67	1286.97	1266.32
4	1286.97	1266.32	1265.87
5	1266.32	1265.87	1265.87* Convergence

$$T_i = 1265.87 \text{ for } C_p(T_i) = 0.2567$$

B. Newton's Method¹⁶:

Newton's method requires a single initial value for temperature, T_0 , and the first derivative of the polynomial function, $F(T_i) = 0$. Newton's method tends to be sensitive to the T_0 selection, the closer T_0 is to the root, T_i , the more rapid it converges. For the polynomials presented, Newton's method generally converges without problems. It is recommended that the initial temperature value, T_0 , be selected mid-range between the polynomial valid temperature limits.

Algorithm: Given $F(T_i) = 0$ and a starting value, T_0

For $n = 0, 1, 2, \dots$ until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - F(T_n)/F'(T_n)$$

For the special case of using a second degree polynomial from Appendix A, Newton's method reduces to the following:

For $n = 0, 1, 2, \dots$ until satisfied, do

$$\text{Calculate } T_{n+1} = T_n - \frac{B(0) - (PV) + B(1)T_n + B(2)T_n^2}{B(1) + 2B(2)T_n}$$

C) Fixed Point Iteration:¹⁶

Fixed point iteration tends to converge the slowest of the three methods discussed. It does, however, provide the user with the function definition. Given the function, $F(T_i) = 0$, the user defines an iterative function, $T = g(T_i)$, such that the solution of the iterative function is also the solution to $F(T_i) = 0$.

Example: Given $F(T_i) = 0 = B(0) + B(1)T_i + B(2)T_i^2 - (PV)$

$$\text{Then } T_i = g_i(T) = \frac{(PV) - B(2)T_i^2 - B(0)}{B(1)}$$

$$\text{Or } T_i = \left(\frac{(PV) - B(0) - B(1)T_i}{B(2)} \right)^{1/2}$$

Algorithm: Given $F(T_i) = 0$, a derived iterative function $g(T)$, and a single starting point, T_0

For $n = 0, 1, 2, \dots$ until satisfied, do

Calculate $T_{n+1} = g(T_n)$

VI. CONCLUSIONS

Within the constraints of a single independent variable (the absolute temperature), it is possible to calculate thermodynamic and transport properties of a large variety of gases accurately. The accuracy of the polynomial results is generally within $\pm 0.5\%$ of the original tabular data. Since interpolation is "build-in", the effort is often no more time consuming than that of reading conventional tabular forms. The inverse problem, namely that of finding the temperature corresponding to a given property, can also be accurately carried out with the information given in this report.

Extrapolation beyond the established valid temperature range is possible but the accuracy of duplication of the property is dubious and cannot be quantified in most cases. The polynomials, however, do allow for a convenient "first guess" in most instances.

It is believed that the combination of simple polynomial representations with the technique of nested multiplication utilized in a modern electronic calculator will make the Gas Tables and other standard works obsolete in form. Integration and differentiation of the polynomials is, moreover, straightforward and virtually risk free so that they are attractive forms for numerical work, particularly with ideal gases. The advantages of simple polynomial representations become vividly clear when other correlation-equation forms are used, see for example the form of the viscosity given in Ref. 5 or 17.

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APPENDIX A
TABLE A-I
SUMMARY OF CONTENTS

SPECIFIC HEAT AT CONSTANT PRESSURE
FOR GASEOUS ELEMENTS AND COMPOUNDS

<u>NAME</u>	<u>FORMULA</u>	<u>AT.WT/ MOL WT</u>	<u>GAS CONST</u>	<u>APP A PAGE</u>
Acetone	C ₃ H ₆ O	58.081	143.150	A-1
Acetylene	C ₂ H ₂	26.038	319.312	A-1
Air	-	28.966	287.037	A-1
Ammonia	NH ₃	17.031	488.199	A-2
Argon	Ar	39.948	208.129	A-2
Arsine	AsH ₃	77.946	106.668	A-2
Arsine, Trideuterated	AsD ₃	80.964	102.692	A-2
Benzene	C ₆ H ₆	78.115	106.437	A-3
Boron Fluoride Oxide, Trimeric	(BOF) ₃	137.426	60.500	A-3
Boron Tribromide	BBr ₃	250.538	33.186	A-3
Boron Trichloride	BCl ₃	117.170	70.959	A-4
Boron Trifluoride	BF ₃	67.806	122.619	A-4
Bromine	Br ₂	159.818	52.024	A-4
Bromine (Monatomic)	Br	79.909	104.047	A-5
Bromine Chloride	BrCl	115.362	72.072	A-5
Bromine Fluoride	BrF	98.907	84.062	A-5
Bromine Pentafluoride	BrF ₅	174.901	47.537	A-5
Bromoform	CHBr ₃	252.746	32.896	A-5
Bromomethane	CH ₃ Br	94.944	87.571	A-6
Bromotrichloromethane	CCl ₃ Br	198.279	41.932	A-6
1,3-Butadiene	(CH ₂ CH) ₂	54.092	153.706	A-6
iso-Butane	i-C ₄ H ₁₀	58.124	143.044	A-6
n-Butane	n-C ₄ H ₁₀	58.124	143.044	A-7
1-Butanol	CH ₃ (CH ₂) ₃ OH	74.124	112.168	A-7
2-Butanone	CH ₃ CH ₂ COCH ₃	72.108	115.304	A-7
1-Butene	CH ₂ CHCH ₂ CH ₃	56.108	148.183	A-7
2-Butene	(CH ₃ CH) ₂	56.108	148.183	A-8
cis-2-Butene	(CH ₃ CH) ₂	56.108	148.183	A-8
trans-2-Butene	(CH ₃ CH) ₂	56.108	148.183	A-8
Butyl Ether	[CH ₃ (CH ₂) ₃] ₂ O	130.232	63.842	A-8
1-Butyne	CHCCH ₂ CH ₃	54.092	153.706	A-8
2-Butyne	(CH ₃ C) ₂	54.092	153.706	A-9
Carbon (Atomic)	C	12.0112*	692.217	A-9
Carbon Dioxide	CO ₂	44.010	188.919	A-9
Carbon Disulfide	CS ₂	76.139	109.199	A-10
Carbon Monoxide	CO	28.011	296.828	A-10
Carbon Monosulfide	CS	44.075	188.640	A-10

*Atomic weight of carbon is 12.01115

TABLE A-I
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Carbon Suboxide	C ₃ O ₂	68.032	122.211	A-10
Carbon Tetrabromide	CBr ₄	331.647	25.070	A-10
Carbon Tetrachloride	CCl ₄	153.823	54.051	A-11
Carbonyl Chloride	COClF	82.462	100.826	A-11
Fluoride				
Carbonyl Fluoride	COF ₂	66.007	125.961	A-11
Carbonyl Sulfide	COS	60.075	138.400	A-11
Chlorine	Cl ₂	70.906	117.258	A-12
Chlorine (Monatomic)	Cl	35.453	234.517	A-12
Chlorine Dioxide	ClO ₂	67.452	123.263	A-12
Chlorine Fluoride	ClF	54.451	152.692	A-12
Chlorine Monoxide	Cl ₂ O	86.905	95.671	A-13
Chlorine Oxide	ClO	51.452	161.592	A-13
Chlorine Trifluoride	ClF ₃	92.448	89.935	A-13
Chlorodifluoromethane	CHClF ₂	86.469	96.154	A-13
(FREON-22)				
Chlorodifluoromethane, CDClF ₂		87.475	95.048	A-14
Monodeuterated				
Chloroform	CHCl ₃	119.378	69.647	A-14
Chlorofluoromethane	CH ₂ ClF	68.478	121.415	A-14
Chloromethylidyne	CCl	47.464	175.171	A-15
Chlorosilane	SiH ₃ Cl	66.563	124.909	A-15
Chlorotrifluoro-	CClF ₃	104.459	79.594	A-15
methane (FREON-13)				
Cumene	C ₆ H ₅ CH(CH ₃) ₂	120.196	69.173	A-15
Cyanogen	(CN) ₂	52.036	159.781	A-15
Cyanogen Chloride	CNCI	61.471	135.256	A-16
Cyclohexane - See Hexane				
Cyclopropane - See Propane				
n-Decane	C ₁₀ H ₂₂	142.287	58.434	A-16
n-Deuterium	D ₂	4.028	2064.131	A-16
Deuterium (monatomic)	D	2.014	4128.262	A-17
Dibromomethane	CH ₂ Br ₂	173.845	47.826	A-17
Dichlorodifluoro-	CCl ₂ F ₂	120.914	68.762	A-17
methane (FREON-12)				
1,1-Dichloro-1-	CH ₃ CFCl ₂	116.951	71.093	A-17
fluoroethane				
Dichlorofluoromethane	CHCl ₂ F	102.924	80.782	A-17
(FREON-21)				
Dichlorofluoromethane, CDCl ₂ F		103.930	80.000	A-18
Monodeuterated				
Dichloromethane	CH ₂ Cl ₂	84.933	97.893	A-18
1,1-Dichlorotetra-	CCl ₂ FCF ₃	170.922	48.644	A-18
fluoroethane				

TABLE A-I
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Dichlorotetrafluoroethane (FREON-114)	C ₂ Cl ₂ F ₄	170.922	48.644	A-18
2,2-Dichloro-1,1,1-trifluoroethane	F ₃ CCHCl ₂	152.931	54.366	A-18
1,1-Difluoroethylene	CH ₂ CF ₂	64.035	129.840	A-19
Difluoromethane	CH ₂ F ₂	52.024	159.817	A-19
Dimethylamine	(CH ₃) ₂ NH	45.085	184.415	A-19
2,2-Dimethylbutane	CH ₃ CH ₂ C(CH ₃) ₃	86.178	96.478	A-19
2,3-Dimethylbutane	[(CH ₃) ₂ CH] ₂	86.178	96.478	A-19
2,3-Dimethylhexane	(CH ₃) ₂ CHCH(CH ₃)(CH ₂) ₂ CH ₃	114.233	72.784	A-20
3,4-Dimethylhexane	[CH(CH ₃)CH ₂ CH ₃] ₂	114.233	72.784	A-20
Dimethylpropane	C(CH ₃) ₄	72.151	115.234	A-20
Dipropylene Glycol	(CH ₃ CHOHCH ₂) ₂ O	134.177	61.965	A-20
Dodecane	CH ₃ (CH ₂) ₁₀ CH ₃	170.341	48.810	A-20
Ethane	C ₂ H ₆	30.070	276.498	A-21
Ethane, Hexadeuterated	C ₂ D ₆	36.106	230.273	A-21
Ethanethiol	C ₂ H ₅ SH	62.134	133.812	A-21
Ethyl Acetate	CH ₃ COOCH ₂ CH ₃	88.107	94.366	A-21
Ethyl Alcohol	C ₂ H ₅ OH	46.070	180.473	A-22
Ethylbenzene	C ₆ H ₅ C ₂ H ₅	106.169	78.312	A-22
Ethyl Ether	C ₄ H ₁₀ O	74.124	112.168	A-22
Ethylene	C ₂ H ₄	28.054	296.367	A-22
Ethylene Oxide	(CH ₂) ₂ O	44.054	188.732	A-23
3-Ethylhexane	(CH ₃ CH ₂) ₂ CH(CH ₂) ₂ CH ₃	114.233	72.784	A-23
3-Ethyl-2-methylpentane	(CH ₃) ₂ CHCH(C ₂ H ₅) ₂	114.233	72.784	A-23
3-Ethyl-3-methylpentane	(CH ₃ CH ₂) ₃ CCH ₃	114.233	72.784	A-23
Fluorine	F ₂	37.997	218.816	A-24
Fluorine (monatomic)	F	18.9984	437.633	A-24
Fluoroethane	CH ₃ CH ₂ F	48.061	172.997	A-24
Fluoroethylene	CH ₂ CHF	46.045	180.571	A-24
Fluoroform, Monodeut.	CF ₃ D	71.020	117.070	A-25
Fluoromethane	CH ₃ F	34.033	244.298	A-25
Formaldehyde	HCHO	30.026	276.899	A-25
Formyl	HCO	29.019	286.518	A-25
Furan	C ₄ H ₄ O	68.076	122.133	A-25
Helium	He	4.003	2077.022	A-26
n-Heptane	C ₇ H ₁₆	100.206	82.973	A-26
Hexafluoroethane	(CF ₃) ₂	138.013	60.243	A-26
n-Hexane	C ₆ H ₁₄	86.178	96.478	A-26

TABLE A-I
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Cyclohexane	C ₆ H ₁₂	84.163	98.789	A-27
Hydrazine	N ₂ H ₄	32.045	259.455	A-27
Hydrobromic Acid	HBr	80.917	102.751	A-27
Hydrocyanic Acid	HCN	27.026	307.644	A-27
Hydrofluoric Acid	HF	20.006	415.584	A-28
Hydrofluoric Acid, Monodeuterated	DF	21.012	395.686	A-28
Hydrogen	H ₂	2.016	4124.289	A-28
Hydrogen (Monatomic)	H	1.008	8248.579	A-29
Hydrogen, Monodeut.	HD	3.022	2751.291	A-29
Hydrogen Chloride	HCl	36.461	228.033	A-29
Hydrogen Iodide	HI	127.912	65.000	A-29
Hydrogen Peroxide	H ₂ O ₂	34.015	244.433	A-29
Hydrogen Sulfide	H ₂ S	34.080	243.965	A-30
Hydrogen Sulfide, Dideuterated	D ₂ S	36.092	230.365	A-30
Hydrogen Sulfide, Ditritiated	T ₂ S	38.098	218.235	A-30
Hydrogen Sulfide, Monodeuterated	HDS	35.086	236.970	A-30
Hydrogen Sulfide, Monodeut/monotrit.	DTS	37.095	224.136	A-30
Hydrogen Sulfide, Monotritiated	HTS	36.089	230.384	A-31
Hydroxyl	OH	17.007	488.866	A-31
Iodine	I ₂	253.809	32.758	A-31
Iodine (monatomic)	I	126.9044	65.516	A-31
Iodine Bromide	IBr	206.813	40.202	A-31
Iodine Chloride	ICl	162.357	51.210	A-31
Iodine Fluoride	IF	145.903	56.985	A-32
Iodine Heptafluoride	IF ₇	259.893	31.991	A-32
Iodine Pentafluoride	IF ₅	221.896	37.469	A-32
Iodomethane	CH ₃ I	141.939	58.577	A-32
Isoprene	CH ₂ C(CH ₃) ₂ CHCH ₂	68.120	122.055	A-32
Ketene	H ₂ CCO	42.038	197.783	A-33
Krypton	Kr	83.80	99.216	A-33
Mesitylene	C ₆ H ₃ (CH ₃) ₃	120.196	69.173	A-33
Methane	CH ₄	16.043	518.251	A-33
Methane, Dideuterated	CH ₂ D ₂	18.055	460.497	A-34
Methane, Dideut, Ditrit.	CD ₂ T ₂	22.073	376.671	A-34
Methane, Ditritiated	CH ₂ T ₂	20.061	414.450	A-34
Methane, Monodeut.	CH ₃ D	17.049	487.670	A-34

TABLE A-I
(CONT.)

NAME	FORMULA	AT. WT/ MOL WT	GAS CONST	APP A PAGE
Methane, Monodeut., Tritritiated	CD ₃ T	23.076	360.299	A-34
Methane, Monotrit.	CH ₃ T	18.052	460.575	A-34
Methane, Tetradeut.	CD ₄	20.067	414.325	A-35
Methane, Tetratrit.	CT ₄	24.079	345.291	A-35
Methane, Trideut.	CHD ₃	19.061	436.193	A-35
Methane, Trideut., Monotritiated	CD ₃ T	21.070	394.602	A-35
Methane, Tritriated	CHT ₃	22.070	376.723	A-35
Methanethiol	CH ₃ SH	48.107	172.830	A-35
Methyl	CH ₃	15.035	552.995	A-36
Methyl Acetate	CH ₃ COOCH ₃	74.080	112.234	A-36
Methyl Alcohol	CH ₃ OH	32.042	259.478	A-36
Methylamine	CH ₃ NH ₂	31.058	267.706	A-36
2-Methylbutane	(CH ₃) ₂ CHCH ₂ CH ₃	72.151	115.234	A-36
2-Methyl-2- butanol	(CH ₃) ₂ COHCH ₂ CH ₃	88.151	94.319	A-37
3-Methyl-1- butanol	(CH ₃) ₂ CH(CH ₂) ₂ OH	88.151	94.319	A-37
3-Methyl-1-butyne	(CH ₃) ₂ CHCCH	68.120	122.055	A-37
Methyl Chloride	CH ₃ Cl	50.488	164.679	A-37
Methyl Cyanide	CH ₃ CN	41.053	202.527	A-38
Methyl Ether	(CH ₃) ₂ O	46.070	180.473	A-38
Methylhydrazine	CH ₃ NHNH ₂	46.072	180.462	A-38
Methylidyne	CH	13.019	638.624	A-38
Methyl Isocyanide	CH ₃ NC	41.053	202.527	A-38
2-Methylpentane	(CH ₃) ₂ CH(CH ₂) ₂ CH ₃	86.178	96.478	A-39
3-Methylpentane	[CH ₃ CH ₂] ₂ CH(CH ₃)	86.178	96.478	A-39
4-Methyl-2- pentanone	CH ₃ COCH ₂ CH(CH ₃) ₂	100.162	83.009	A-39
2-Methyl-1- propanol	(CH ₃) ₂ CHCH ₂ OH	74.124	112.168	A-39
2-Methyl-2-propanol	(CH ₃) ₃ COH	74.124	112.168	A-40
2-Methylpropene	(CH ₃) ₂ CCH ₂	56.108	148.183	A-40
Methyl Sulfide	(CH ₃) ₂ S	62.134	133.812	A-40
Neon	Ne	20.183	411.947	A-40
Nitric Oxide	NO	30.006	277.088	A-40
Nitrogen	N ₂	28.013	296.798	A-41
Nitrogen (Monatomic)	N	14.0067	593.596	A-41
Nitrous Oxide	N ₂ O	44.013	188.907	A-41
n-Nonane	C ₉ H ₂₀	128.260	64.824	A-42
n-Octane	C ₈ H ₁₈	114.233	72.784	A-42

TABLE A-I
(CONT.)

NAME	FORMULA	AT.WT/ MOL WT	GAS CONST	APP A PAGE
Oxygen	O ₂	31.999	259.832	A-42
Oxygen (Monatomic)	O	15.9994	519.664	A-43
Oxygen Fluoride	OF ₂	53.996	153.980	A-43
n-Pentane	C ₅ H ₁₂	72.151	115.234	A-44
1-Pentanol	CH ₃ (CH ₂) ₄ OH	88.151	94.319	A-44
3-Pentanone	(C ₂ H ₅) ₂ CO	86.135	96.527	A-44
1-Pentene	CH ₂ CH(CH ₂) ₂ CH ₃	70.135	118.547	A-45
1-Pentyne	HCCCH ₂ CH ₂ CH ₃	68.120	122.055	A-45
2-Pentyne	CH ₃ CCCH ₂ CH ₃	68.120	122.055	A-45
Phosgene	COCl ₂	98.917	84.054	A-45
Phosphine	PH ₃	33.998	244.555	A-46
Phosphine, Trideut.	PD ₃	37.016	224.615	A-46
Phosphorus Trichloride	PCl ₃	137.333	60.541	A-46
Phosphorus Trifluoride	PF ₃	87.969	94.514	A-46
Propadiene	C(CH ₂) ₂	40.065	207.519	A-46
Propane	C ₃ H ₈	44.097	188.545	A-47
Cyclopropane	C ₃ H ₈	44.097	188.545	A-47
1,2-Propanediol	CH ₃ CHOHCH ₂ OH	76.096	109.261	A-47
1-Propanol	CH ₃ (CH ₂) ₂ OH	60.097	138.349	A-47
2-Propanol	(CH ₃) ₂ CHOH	60.097	138.349	A-48
Propylbenzene	C ₆ H ₅ (CH ₂) ₂ CH ₃	120.196	69.173	A-48
Propyl Ether	[CH ₃ (CH ₂) ₂] ₂ O	102.178	81.371	A-48
Propyne	CH ₃ CCH	40.065	207.519	A-48
Silane	SiH ₄	32.118	258.869	A-49
Silicon Tetrachloride	SiCl ₄	169.898	48.937	A-49
Silicon Tetrafluoride	SiF ₄	104.080	79.884	A-49
Styrene	C ₆ H ₅ CHCH ₂	104.153	79.828	A-49
Sulfur	S ₂	64.128	129.652	A-49
Sulfur (monatomic)	S	32.064	259.304	A-49
Sulfur Dichloride	SCl ₂	102.970	80.745	A-50
Sulfur Difluoride	SF ₂	70.061	118.673	A-50
Sulfur Dioxide	SO ₂	64.063	129.784	A-50
Sulfur Hexafluoride	SF ₆	146.054	56.926	A-50
Sulfur Monochloride	S ₂ Cl ₂	135.034	61.572	A-50
Sulfur Monoxide	SO	48.063	172.987	A-50
Sulfur Tetrafluoride	SF ₄	108.058	76.943	A-51
Sulfur Trioxide	SO ₃	80.062	103.848	A-51
Sulfuryl Fluoride	SO ₂ F ₂	102.060	81.465	A-51
Thionyl Chloride	SOCl ₂	118.969	69.886	A-51
Thionyl Fluoride	SOF ₂	86.060	96.611	A-51
Thiophosgene	CSCl ₂	114.981	72.310	A-51
Toluene	C ₇ H ₈	92.142	90.234	A-52
1,1,1-Trichloroethane	CH ₃ CCl ₃	133.405	62.324	A-52

TABLE A-I
(CONT.)

NAME	FORMULA	AT WT/ MOL WT	GAS CONST	APP A PAGE
Trichlorofluoro- methane (FREON-11)	CCl ₃ F	137.369	60.526	A-52
Trichlorotrifluoro- ethane (FREON-113)	C ₂ Cl ₃ F ₃	187.377	44.372	A-53
Trichlorosilane	SiHCl ₃	135.453	61.382	A-53
1,1,1-trichloro-2,2,2- trifluoroethane	CF ₃ CCl ₃	187.377	44.372	A-53
1,1,1-Trifluoroethane	CH ₃ CF ₃	84.041	98.931	A-53
Trifluoroiodomethane	CF ₃ I	195.911	42.439	A-54
Trimethylamine	(CH ₃) ₃ N	59.112	140.654	A-54
2,3,4-Trimethyl-[$(CH_3)_2CH$] ₂ CHCH ₃		114.233	72.784	A-54
Water	H ₂ O	18.015	461.513	A-54
Water, Dideuterated	D ₂ O	20.027	415.147	A-55
Xenon	Xe	131.30	63.323	A-55
m-Xylene	C ₆ H ₄ (CH ₃) ₂	106.169	78.312	A-55
o-Xylene	C ₆ H ₄ (CH ₃) ₂	106.169	78.312	A-56
p-Xylene	C ₆ H ₄ (CH ₃) ₂	106.169	78.312	A-56

APPENDIX A
FORMAT EXAMPLE

The equations presented are for gaseous Acetylene (ideal gas)

The polynomial equation to calculate the specific heat (C_p) in J/Kg K as a function of temperature (Kelvin)

Formula	Valid temperature range
ACETYLENE - Ideal gas	C_2H_2
	275-755K

$$C_p(T) = 399.896066 + 6.226492T - 7.433125E-03T^2 + 3.4974695E-06T^3$$

$$C_p(275) = 1622.79 \quad C_p(450) = 2015.32 \quad C_p(755) = 2369.03$$

std error est = 0.111 max error est = 1.0

$$C_p(T) = 1321.969854 + 1.9041159T - 7.913804E-04T^2 + 1.403319E-07T^3$$

$$C_p(755) = 2368.87 \quad C_p(1000) = 2575.04 \quad C_p(1365) = 2803.47$$

std error est = 0.111 max error est = 1.0

$$T(C_p) = 1717.26917 - 1.9064232C_p + 6.3328193E-04C_p^2$$

$$T(1622.79) = 291 \quad T(2368.87) = 755 \quad T(2803.47) = 1350$$

std error est = 5 max error est = 15

standard (or average) error estimate is ± 5 degrees Kelvin

The polynomial equation to calculate temperature (Kelvin) as a function of specific heat (C_p) in J/Kg K

Using the polynomial presented, the calculated specific heat at 755K is 2369.03 J/Kg K.

Over the temperature range noted, the maximum error est is ± 1 J/Kg K.

FIGURE A-1

APPENDIX A

SPECIFIC HEAT AT CONSTANT PRESSURE FOR GASEOUS ELEMENTS AND COMPOUNDS

ACETONE - Ideal gas C₃H₆O 275-1365K

$$C_p(T) = 345.6240845 + 3.1344046T + 9.000608E-04T^2 - 1.9981015E-06T^3 \\ - 7.2481823E-10T^4 + 1.757756E-12T^5 - 5.94192596E-16T^6$$

$$C_p(275) = 1232.46 \quad C_p(700) = 2346.88 \quad C_p(1365) = 3189.13 \\ \text{std error est} = 0.791 \quad \text{max error est} = 1.25$$

275-1365K

$$T(C_p) = -537.70187 + 1.08064298C_p - 4.673706E-04C_p^2 + 9.857246E-08C_p^3$$

$$T(1232.46) = 269 \quad T(2346.88) = 698 \quad T(3189.13) = 1352$$

- std error est = 3 max error est = 13

ACETYLENE - Ideal gas C₂H₂ 275-755K

$$C_p(T) = 399.896066 + 6.226492T - 7.433125E-03T^2 + 3.4974695E-06T^3$$

$$C_p(275) = 1622.79 \quad C_p(450) = 2015.32 \quad C_p(755) = 2369.03 \\ \text{std error est} = 0.111 \quad \text{max error est} = 1.0$$

755-1365K

$$C_p(T) = 1321.969854 + 1.9041159T - 7.913804E-04T^2 + 1.403319E-07T^3$$

$$C_p(755) = 2368.87 \quad C_p(1000) = 2575.04 \quad C_p(1365) = 2803.47 \\ \text{std error est} = 0.111 \quad \text{max error est} = 1.0$$

275-1365K

$$T(C_p) = 1717.26917 - 1.9064232C_p + 6.3328193E-04C_p^2$$

$$T(1622.79) = 291 \quad T(2368.87) = 755 \quad T(2803.47) = 1350$$

- std error est = 5 max error est = 15

AIR - Ideal gas 100-590K

$$C_p(T) = 1022.5294853 - 0.1758625T + 4.020605E-04T^2 - 4.8640623E-08T^3$$

$$C_p(100) = 1008.92 \quad C_p(350) = 1008.14 \quad C_p(590) = 1048.74 \\ \text{std error est} = 0.012 \quad \text{max error est} = 0.025$$

590-1365K

$$C_p(T) = 928.911894 + 0.0897769T + 3.2460657E-04T^2 - 2.62542E-07T^3$$

$$+ 5.99901E-11T^4$$

$$C_p(590) = 1048.22 \quad C_p(1000) = 1140.74 \quad C_p(1365) = 1196.81 \\ \text{std error est} = 0.22 \quad \text{max error est} = 0.5$$

590-1365K

$$T(C_p) = -100444.9907 + 275.16644C_p - 0.253212C_p^2 + 7.885293E-05C_p^3$$

$$T(1048.22) = 588 \quad T(1140.74) = 998 \quad T(1196.81) = 1361$$

$$\text{std error est} = 1.5 \quad \text{max error est} = 4$$

Note: For T(C_p) calculations below 590K use the iterative procedures discussed in Section 5 and the following polynomial: 100-590K,
 $C_p(T) = 1021.17215 - 0.1603904T + 3.5182525E-04T^2.$

AIR - Real gas

255-865K

$$Cp(T) = 1052.71406 - 0.3745355T + 8.361477E-04T^2 - 3.32111E-07T^3 - 4.683905E-11T^4$$

$$Cp(255) = 1005.87 \quad Cp(560) = 1042.26 \quad Cp(865) = 1113.2$$

std error est = 0.17 max error est = 0.4

Note: For T(Cp) calculations use the iterative procedures discussed in Section 5 and the following polynomial: 255-865K, $Cp(T) = 996.831581 - 0.0322256T + 2.0181265E-04T^2$.

AMMONIA - Ideal gas NH₃ 220-590K

$$Cp(T) = 1948.475605 - 0.81912827T + 5.424779E-03T^2 - 3.60715E-06T^3$$
$$Cp(220) = 1992.42 \quad Cp(400) = 2257.93 \quad Cp(590) = 2612.72$$

std error est = 0.12 max error est = 1.0

$$Cp(T) = 2124.419956 - 1.746889T + 8.22758E-03T^2 - 8.855634E-06T^3 + 4.420294E-09T^4 - 8.734964E-13T^5$$

$$Cp(590) = 2612.19 \quad Cp(1000) = 3296.27 \quad Cp(1365) = 3753.45$$

std error est = 0.36 max error est = 1.0

$$T(Cp) = -8836.6068 + 10.54741Cp - 4.154804E-03Cp^2 + 5.737145E-07Cp^3$$
$$T(1992.42) = 222 \quad T(2257.93) = 401 \quad T(2612.72) = 591$$

std error est = 0.8 max error est = 2.0

$$T(Cp) = -2501.9985 + 2.45231Cp - 7.299265E-04Cp^2 + 9.350415E-08Cp^3$$
$$T(2612.19) = 590 \quad T(3296.27) = 999 \quad T(3753.45) = 1364$$

std error est = 0.5 max error est = 2.0

ARGON - Ideal gas Ar 0-6000K

Cp = 520.34 (constant)

ARSINE AsH₃ 300-1000K

$$Cp(T) = 347.13902 + 0.231073T + 1.309066E-03T^2 - 1.577571E-06T^3 + 5.450638E-10T^4$$

$$Cp(300) = 496.1 \quad Cp(600) = 686.93 \quad Cp(1000) = 854.77$$

std error est = 1.13 max error est = 2.0

$$T(Cp) = -1935.0966 + 9.24965Cp - 1.33801E-02Cp^2 + 7.69057E-06Cp^3$$
$$T(496.1) = 300 \quad T(686.93) = 598 \quad T(854.77) = 998$$

std error est = 3.3 max error est = 5.0

ARSINE, Trideuterated AsD₃ 300-1000K

$$Cp(T) = 245.545853 + 1.09726T - 3.84163E-05T^2 - 8.056253E-07T^3 + 4.042793E-10T^4$$

$$Cp(300) = 552.79 \quad Cp(600) = 768.45 \quad Cp(1000) = 903.04$$

ARSINE, Trideuterated (continued)

std error est = 0.43 max error est = 2.0

$$\begin{aligned} T(Cp) &= 8581.361485 - 52.568517Cp + 0.121435Cp^2 - 1.22502E-04Cp^3 \\ &\quad + 4.6727183E-08Cp^4 \\ T(552.79) &= 300 \quad T(768.45) = 599 \quad T(903.04) = 1000 \\ \text{std error est} &= 1.3 \quad \text{max error est} = 3.0 \end{aligned}$$

 BENZENE - Ideal gas C₆H₆ 275-1365K

Cp(T) = -297.4345373 + 4.42278708T + 2.810036E-03T² - 1.136955E-05T³

$$\begin{aligned} &\quad + 1.1190287E-08T^4 - 4.8717996E-12T^5 + 8.019155E-16T^6 \\ Cp(275) &= 951.57 \quad Cp(800) = 2415.38 \quad Cp(1365) = 3008.37 \\ \text{std error est} &= 0.67 \quad \text{max error est} = 1.3 \end{aligned}$$

$$\begin{aligned} T(Cp) &= 392.0602 - 0.648326Cp + 8.326166E-04Cp^2 - 3.4749E-07Cp^3 \\ &\quad + 5.9114275E-11Cp^4 \\ T(951.57) &= 278 \quad T(2415.38) = 799 \quad T(3008.37) = 1358 \\ \text{std error est} &= 1.6 \quad \text{max error est} = 7 \end{aligned}$$

BENZENE - Real gas 300-600K

Cp(T) = -283.22595 + 5.300935T - 2.4209348E-03T²

$$\begin{aligned} Cp(300) &= 1089.17 \quad Cp(450) = 1611.96 \quad Cp(600) = 2025.8 \\ \text{std error est} &= 0.9 \quad \text{max error est} = 1.5 \end{aligned}$$

$$\begin{aligned} T(Cp) &= 129.444998 + 0.07207415Cp + 7.8699477E-05Cp^2 \\ T(1089.17) &= 301 \quad T(1611.96) = 450 \quad T(2025.8) = 598 \end{aligned}$$

BORON FLUORIDE OXIDE, (BOF)₃ 300-500K

Trimeric

$$\begin{aligned} Cp(T) &= 79.2504 + 3.2856459T - 2.3282776E-03T^2 \\ Cp(300) &= 855.4 \quad Cp(400) = 1021 \quad Cp(500) = 1140 \\ \text{std error est} &= 0.6 \quad \text{max error est} = 1.0 \end{aligned}$$

$$\begin{aligned} T(Cp) &= 505.381375 - 0.9481142Cp + 8.275349E-04Cp^2 \\ T(855.4) &= 300 \quad T(1021) = 400 \quad T(1140) = 500 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

BORON TRIBROMIDE BBr₃ 300-1000K

Cp(T) = 140.1554722 + 0.71322266T - 1.1636584E-03T² + 9.112207E-07T³

$$\begin{aligned} &\quad - 2.780408E-10T^4 \\ Cp(300) &= 271.74 \quad Cp(650) = 312.72 \quad Cp(1000) = 322.9 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

Note: For T(Cp) calculations use the iterative procedures discussed
 in Section 5 and: Cp(T) = 212.708133 + 0.24356T - 1.35451E-04T².

BORON TRICHLORIDE BCl_3 100-1500K

$$\begin{aligned} \text{Cp}(T) &= 188.655802 + 1.888567T - 3.184433E-03T^2 + 2.8712E-06T^3 \\ &\quad - 1.3291673E-09T^4 + 2.474797E-13T^5 \\ \text{Cp}(100) &= 348.8 \quad \text{Cp}(800) = 668.19 \quad \text{Cp}(1500) = 697.22 \\ \underline{\text{std error est}} &= 0.5 \quad \underline{\text{max error est}} = 1.0 \end{aligned}$$

BORON TRIFLUORIDE BF_3 145-645K

Ideal gas

$$\begin{aligned} \text{Cp}(T) &= 298.65561 + 1.865263T - 1.3085604E-03T^2 + 1.995E-07T^3 \\ \text{Cp}(145) &= 542.21 \quad \text{Cp}(400) = 848.16 \quad \text{Cp}(645) = 1010.89 \\ \underline{\text{std error est}} &= 0.24 \quad \underline{\text{max error est}} = 1.0 \end{aligned}$$

$$\begin{aligned} \text{Cp}(T) &= 466.430362 + 1.331415T - 8.914198E-04T^2 + 2.12377E-07T^3 \\ \text{Cp}(645) &= 1011.33 \quad \text{Cp}(1000) = 1118.80 \quad \text{Cp}(1365) = 1163.04 \\ \underline{\text{std error est}} &= 0.11 \quad \underline{\text{max error est}} = 1.0 \end{aligned}$$

$$\begin{aligned} \text{T(Cp)} &= 1438.87308 - 8.75606\text{Cp} + 0.020047\text{Cp}^2 - 1.908134E-05\text{Cp}^3 \\ &\quad + 6.971855E-09\text{Cp}^4 \\ \text{T}(542.21) &= 146 \quad \text{T}(848.16) = 399 \quad \text{T}(1010.89) = 642 \\ \underline{\text{std error est}} &= 0.6 \quad \underline{\text{max error est}} = 3.0 \end{aligned}$$

$$\begin{aligned} \text{T(Cp)} &= -180147.73 + 519.93406\text{Cp} - 0.5005\text{Cp}^2 + 1.613357E-04\text{Cp}^3 \\ \text{T}(1011.33) &= 653 \quad \text{T}(1118.80) = 1009 \quad \text{T}(1163.04) = 1362 \\ \underline{\text{std error est}} &= 5.2 \quad \underline{\text{max error est}} = 12 \end{aligned}$$

BROMINE - Ideal gas Br_2 200-590K

$$\begin{aligned} \text{Cp}(T) &= 175.261725 + 0.304817T - 5.66955E-04T^2 + 3.5797E-07T^3 \\ &\quad + 1.30779E-11T^4 \\ \text{Cp}(200) &= 216.43 \quad \text{Cp}(400) = 229.72 \quad \text{Cp}(590) = 232.85 \\ \underline{\text{std error est}} &= 1.2E-02 \quad \underline{\text{max error est}} = 0.2 \end{aligned}$$

$$\begin{aligned} \text{Cp}(T) &= 223.7002 + 2.231436E-02T - 1.335276E-05T^2 + 3.0736E-09T^3 \\ \text{Cp}(590) &= 232.85 \quad \text{Cp}(1000) = 235.74 \quad \text{Cp}(1365) = 237.097 \\ \underline{\text{std error est}} &= 9.9E-03 \quad \underline{\text{max error est}} = 0.2 \end{aligned}$$

$$\begin{aligned} \text{T(Cp)} &= -649483.9088 + 2282.92562\text{Cp} + 48.1995412\text{Cp}^2 - 0.335799\text{Cp}^3 \\ &\quad + 5.93457E-04\text{Cp}^4 \\ \text{T}(216.43) &= 183 \quad \text{T}(229.72) = 402 \quad \text{T}(232.85) = 589 \\ \underline{\text{std error est}} &= 6.0 \quad \underline{\text{max error est}} = 17.0 \end{aligned}$$

$$\begin{aligned} \text{T(Cp)} &= 1327415.6666 - 11467.00468\text{Cp} + 24.77498\text{Cp}^2 \\ \text{T}(232.85) &= 601 \quad \text{T}(235.74) = 1013 \quad \text{T}(237.097) = 1348 \\ \underline{\text{std error est}} &= 7.0 \quad \underline{\text{max error est}} = 21 \end{aligned}$$

BROMINE (Monatomic) B 250-1500K

$Cp(T) = 264.48344899 - 2.672822E-02T + 4.013018E-05T^2 - 1.04915E-08T^3$
 $Cp(250) = 260.14 \quad Cp(900) = 265.29 \quad Cp(1500) = 279.28$
std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed
in Section 5 and the following eqn: 250-1500K, $Cp(T) = 260.01432$
 $- 5.58942E-03T + 1.263795E-05T^2$.

BROMINE CHLORIDE BrCl 250-1500K

$Cp(T) = 194.97556 + 0.764857T - 2.058934E-03T^2 + 3.0416852E-06T^3$
 $- 2.5048785E-09T^4 + 1.07526E-12T^5 - 1.870628E-16T^6$
 $Cp(250) = 296.25 \quad Cp(900) = 325.06 \quad Cp(1500) = 328.89$
std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed
in Section 5 and the following eqn: 250-1500K, $Cp(T) = 283.400876$
 $+ 7.585277E-02T - 3.15832E-05T^2$.

BROMINE FLUORIDE BrF 250-1500K

$Cp(T) = 241.432653 + 0.456866T - 6.069283E-04T^2 + 3.694047E-07T^3$
 $- 8.374216E-11T^4$
 $Cp(250) = 323.16 \quad Cp(900) = 375.35 \quad Cp(1500) = 383.94$
std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed
in Section 5 and the following eqn: 250-1500K, $Cp(T) = 266.492708$
 $+ 0.291667T - 2.572893E-04T^2 + 7.705475E-08T^3$.

BROMINE PENTAFLUORIDE BrF₅ 250-1500K

$Cp(T) = -106.97977 + 4.406352T - 1.040336E-02T^2 + 1.362716E-05T^3$
 $- 1.013227E-08T^4 + 3.9961242E-12T^5 - 6.484931E-16T^6$
 $Cp(250) = 521.49 \quad Cp(900) = 733.47 \quad Cp(1500) = 750.86$
std error est = 0.51 max error est = 1.0

BROMOFORM CHBr₃ 100-1500K

$Cp(T) = 142.57457 + 0.651772857T - 5.93501E-04T^2 + 1.831537E-07T^3$
 $Cp(100) = 202.0 \quad Cp(900) = 381.95 \quad Cp(1500) = 403.0$
std error est = 0.01 max error est = 0.1

Note: For T(Cp) calculations, use the iterative procedures discussed
in Section 5 and the equation above.

iso-BUTANE - Real gas (continued)

- std error est = 1.7 - - - - - max error est = 6 -

n-BUTANE n-C₄H₁₀ 265-755K

Ideal gas

$$Cp(T) = 236.65134 + 5.10573T - 4.16089E-04T^2 - 1.1450804E-06T^3$$

$$Cp(265) = 1539.14 \quad Cp(500) = 2542.36 \quad Cp(755) = 3361.49$$

std error est = 0.2 max error est = 1.0

755-1365K

$$Cp(T) = 4401.26486 - 13.90866545T + 3.471109E-02T^2 - 3.45278E-05T^3$$

$$+ 1.619382E-08T^4 - 2.966666E-12T^5$$

$$Cp(755) = 3360.77 \quad Cp(1000) = 3903.04 \quad Cp(1365) = 4436.19$$

std error est = 0.7 max error est = 1.5

265-1365K

$$T(Cp) = -372.95792 + 0.63692878Cp - 1.95552E-04Cp^2 + 3.149068E-08Cp^3$$

$$T(3360.77) = 754 \quad T(3903.04) = 1006 \quad T(4436.19) = 1353$$

- std error est = 3.5 - - - - - max error est = 12 -

1-BUTANOL CH₃(CH₂)₃OH 395-605K

$$Cp(T) = 740069.2476 - 7408.748863T + 29.59687066T^2 - 5.88465E-02T^3$$

$$+ 5.82563958E-05T^4 - 2.297227E-08T^5$$

$$Cp(395) = 2048.05 \quad Cp(500) = 2241.28 \quad Cp(605) = 2555.35$$

std error est = 16.0 max error est = 23.0

Note: This is an extremely poor fit of the tabular data. The max error est of 23 represents an error of 1.2% of the table data.

2-BUTANONE CH₃CH₂COCH₃ 275-1275K

$$Cp(T) = 20.545066 + 7.021058T - 1.15892E-02T^2 + 1.631369E-05T^3$$

$$- 1.31136E-08T^4 + 4.917275E-12T^5 - 5.9919712E-16T^6$$

$$Cp(275) = 1346.65 \quad Cp(800) = 2655.8 \quad Cp(1275) = 3284.96$$

- std error est = 6.6 - - - - - max error est = 12 (0.9%)

1-BUTENE CH₂CHCH₂CH₃ 275-1500K

$$Cp(T) = 139.59317 + 4.97386775T + 1.700397E-03T^2 - 9.414594E-06T^3$$

$$+ 1.0035756E-08T^4 - 4.7956263E-12T^5 + 8.828364E-16T^6$$

$$Cp(275) = 1490.44 \quad Cp(900) = 3352.02 \quad Cp(1500) = 4097.32$$

std error est = 1.12 max error est = 2.5

275-1500K

$$T(Cp) = 739.649 - 1.1519803Cp + 8.633103E-04Cp^2 - 2.397716E-07Cp^3$$

$$+ 2.6524417E-11Cp^4$$

$$T(1490.44) = 277 \quad T(3352.02) = 896 \quad T(4097.32) = 1496$$

- std error est = 3.2 max error est = 6.0 -

2-BUTENE $(CH_3CH)_2$ 300-1000K

$Cp(T) = -53.440476 + 5.5916666T - 2.05714285E-03T^2$
 $Cp(300) = 1438.92 \quad Cp(600) = 2560.99 \quad Cp(1000) = 3481.08$
 $std\ error\ est = 0.23 \quad max\ error\ est = 1.0$
 $T(Cp) = 470.8465 - 0.72122159Cp + 6.591403E-04Cp^2 - 2.020906E-07Cp^3$
 $+ 2.435593E-11Cp^4$
 $T(1438.92) = 300 \quad T(2560.99) = 600 \quad T(3481.08) = 999$
 $std\ error\ est = 1.4 \quad max\ error\ est = 3$

cis-2-BUTENE $(CH_3CH)_2$ 275-1500K

$Cp(T) = 593.119884 - 0.25533449T + 1.75336E-02T^2 - 3.26788E-05T^3$
 $+ 2.844997E-08T^4 - 1.2341584E-11T^5 + 2.139958E-15T^6$
 $Cp(275) = 1313.49 \quad Cp(900) = 3258.39 \quad Cp(1500) = 4054.29$
 $std\ error\ est = 1.3 \quad max\ error\ est = 3.0$
 $T(Cp) = 367.106 - 0.531809Cp + 5.3353694E-04Cp^2 - 1.6407E-07Cp^3$
 $+ 2.0168237E-11Cp^4$
 $T(1313.49) = 277 \quad T(3258.39) = 896 \quad T(4054.29) = 1496$
 $std\ error\ est = 3.5 \quad max\ error\ est = 5.0$

trans-2-BUTENE $(CH_3CH)_2$ 275-1500K

$Cp(T) = 725.45579 + 0.662269T + 1.2774909E-02T^2 - 2.40152E-05T^3$
 $+ 2.06644E-08T^4 - 8.859714E-12T^5 + 1.5207345E-15T^6$
 $Cp(275) = 1479.15 \quad Cp(900) = 3296.61 \quad Cp(1500) = 4068.29$
 $std\ error\ est = 1.2 \quad max\ error\ est = 3.5$
 $T(Cp) = 525.129 - 0.865304Cp + 7.3369042E-04Cp^2 - 2.134057E-07Cp^3$
 $+ 2.4521456E-11Cp^4$
 $T(1479.15) = 277 \quad T(3296.61) = 897 \quad T(4068.29) = 1496$
 $std\ error\ est = 3 \quad max\ error\ est = 5.$

BUTYL ETHER $[CH_3(CH_2)_3]_2O$ 275-1275K

$Cp(T) = 2220.96497 - 15.85878T + 8.3621339E-02T^2 - 1.752393E-04T^3$
 $+ 1.899729E-07T^4 - 1.0442973E-10T^5 + 2.2914465E-14T^6$
 $Cp(275) = 1471.38 \quad Cp(800) = 2929.33 \quad Cp(1275) = 3333.16$
 $std\ error\ est = 9.0 \quad max\ error\ est = 15.0$

1-BUTYNE $CH_3CCH_2CH_3$ 300-1500K

$Cp(T) = 138.2438 + 5.66515T - 4.1092457E-03T^2 + 1.692264E-06T^3$
 $- 3.051742E-10T^4$
 $Cp(300) = 1511.18 \quad Cp(800) = 2781.89 \quad Cp(1500) = 3556.61$
 $std\ error\ est = 0.95 \quad max\ error\ est = 2.0$

CARBON DIOXIDE - Real gas (continued)

T(760.75) = 205 T(1168.2) = 796 T(1310.6) = 1350
std error est = 4.5 max error est = 17
 CARBON DISULFIDE CS₂ 100-1500K

Cp(T) = 234.3967 + 2.083974T - 4.080167E-03T² + 4.899365E-06T³
 - 3.4779E-09T⁴ + 1.329115E-12T⁵ - 2.100283E-16T⁶
 Cp(100) = 406.56 Cp(800) = 754.66 Cp(1500) = 809.08
std error est = 0.9 max error est = 2.0

CARBON MONOXIDE CO 255-1365K

Ideal gas

Cp(T) = 1020.802 + 0.382075T - 2.4945E-03T² + 6.81145E-06T³
 - 7.93722E-09T⁴ + 4.291972E-12T⁵ - 8.903274E-16T⁶
 Cp(255) = 1039.79 Cp(700) = 1113.16 Cp(1365) = 1242.76
 std error est = 0.27 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 255-1365K, Cp(T) = 1060.3 - 0.2338408T + 6.188684E-04T² - 2.584758E-07T³.

CARBON MONOXIDE - Real gas 275-1365K

Cp(T) = 1036.64564 + 0.2738793T - 2.16729E-03T² + 6.279075E-06T³
 - 7.459832E-09T⁴ + 4.072163E-12T⁵ - 8.50011E-16T⁶
 Cp(275) = 1042.02 Cp(700) = 1113.41 Cp(1365) = 1243.06
 std error est = 0.26 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the 3rd degree polynomial in the note above.

CARBON MONOSULFIDE CS 100-1500K

Cp(T) = 695.6713 - 0.590035T + 2.78573E-03T² - 4.25312E-06T³
 + 3.1619707E-09T⁴ - 1.16023E-12T⁵ + 1.6791E-16T⁶
 Cp(100) = 660.58 Cp(800) = 787.89 Cp(1500) = 833.81
std error est = 1.1 max error est = 2.0

CARBON SUBOXIDE C₃O₂ 275-1500K

ln[Cp(T)] = 5.7661716 + 6.399978E-03T - 1.20235687E-05T²
 + 1.16497649E-08T³ - 5.5686458E-12T⁴ + 1.03973134E-15T⁵
 Cp(275) = 924.22 Cp(800) = 1377.47 Cp(1500) = 1533.42
 Note: Cp(T) = exp[fctn(T) above] max error est = 36

CARBON TETRABROMIDE CBr₄ 300-1000K

Cp(T) = 195.977 + 0.3730265T - 3.99407E-04T² + 1.498015E-07T³
 Cp(300) = 275.98 Cp(600) = 308.36 Cp(1000) = 319.4

CARBON TETRABROMIDE (Continued)

std error est = 1.86

max error est = 3.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1000K, Cp(T) = $228.26176 + 0.1975507T - 1.0812615E-04T^2$ - - - - -

CARBON TETRACHLORIDE CCl_4 100-700K

Ideal gas

$$Cp(T) = 104.89579 + 2.318459T - 2.59822E-03T^2 - 2.90876E-06T^3 + 8.5781275E-09T^4 - 5.07917E-12T^5$$

$$Cp(100) = 308.66 \quad Cp(450) = 615.03 \quad Cp(700) = 662.94 \\ std\ error\ est = 0.4 \qquad \qquad \qquad max\ error\ est = 1.0$$

$$Cp(T) = 458.4405 + 0.526876T - 4.11842E-04T^2 + 1.1014289E-07T^3 \\ Cp(700) = 663.23 \quad Cp(1000) = 683.62 \quad Cp(1365) = 690.4 \\ std\ error\ est = 0.2 \qquad \qquad \qquad max\ error\ est = 1.0$$

$$T(Cp) = 4845.83 - 45.40359Cp + \frac{100-700K}{0.158658Cp^2} - 2.40639E-04Cp^3 + 1.362815E-07Cp^4 \\ T(308.66) = 108 \quad T(615.03) = 452 \quad T(662.94) = 686 \\ std\ error\ est = 4.5 \qquad \qquad \qquad max\ error\ est = 14$$

Note: For T(Cp) calculations from 700-1365K, use the iterative procedures discussed in Section 5 and the following eqn: 700-1365K, $Cp(T) = 563.12016 + 0.198424T - 7.78963E-05T^2$ - - - - -

CARBONYL CHLORIDE $COClF$ 100-1500K

FLUORIDE

$$Cp(T) = 309.8366 + 0.908395T + 2.14223E-03T^2 - 7.3825E-06T^3 + 8.468816E-09T^4 - 4.393756E-12T^5 + 8.6745044E-16T^6$$

$$Cp(100) = 415.52 \quad Cp(800) = 884.22 \quad Cp(1500) = 965.61 \\ std\ error\ est = 2.7 \qquad \qquad \qquad max\ error\ est = 4.5$$

CARBONYL FLUORIDE COF_2 100-1500K

$$Cp(T) = 500.9343 - 0.685575T + 9.023284E-03T^2 - 1.958117E-05T^3 + 1.949097E-08T^4 - 9.392863E-12T^5 + 1.769924E-15T^6$$

$$Cp(100) = 504.88 \quad Cp(800) = 1071.45 \quad Cp(1500) = 1195.03 \\ std\ error\ est = 3.9 \qquad \qquad \qquad max\ error\ est = 7.5$$

CARBONYL SULFIDE COS 100-1500K

$$Cp(T) = 383.5831 + 1.008813T + 1.13734E-03T^2 - 5.397317E-06T^3 + 6.74814E-09T^4 - 3.689623E-12T^5 + 7.566326E-16T^6$$

$$Cp(100) = 491.08 \quad Cp(800) = 908.47 \quad Cp(1500) = 1002.78 \\ std\ error\ est = 3.2 \qquad \qquad \qquad max\ error\ est = 6.0$$

CHLORINE - Ideal gas Cl₂ 200-590K

$$Cp(T) = 333.73754 + 0.7763656T - 1.167902E-03T^2 + 6.302785E-07T^3$$

$$Cp(200) = 447.34 \quad Cp(400) = 497.76 \quad Cp(590) = 514.69$$

std error est = 0.15 max error est = 0.5

590-1365K

$$Cp(T) = 459.54857 + 0.1432384T - 9.84775E-05T^2 + 2.443506E-08T^3$$

$$Cp(590) = 514.8 \quad Cp(900) = 526.51 \quad Cp(1365) = 533.73$$

std error est = 0.14 max error est = 0.5

200-590K

$$T(Cp) = -164812.69 + 1056.14056Cp - 2.258534Cp^2 + 1.61435E-03Cp^3$$

$$T(447.34) = 193 \quad T(497.76) = 400 \quad T(514.69) = 581$$

std error est = 4.5 max error est = 12

Note: For T(Cp) calculations from 590-1365K, use the iterative procedures discussed in Section 5 and the following eqn; 590-

$$- 1365K, Cp(T) = 478.47124 + 7.90734E-02T - 2.858817E-05T^2 - - - - -$$

CHLORINE (Atomic) Cl 100-1500K

$$Cp(T) = 603.43652 - 0.43322T + 3.15819E-03T^2 - 7.17812E-06T^3$$

$$+ 7.4774E-09T^4 - 3.716555E-12T^5 + 7.151811E-16T^6$$

$$Cp(100) = 585.23 \quad Cp(800) = 635.29 \quad Cp(1500) = 611.49$$

std error est = 1.4 max error est = 2.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K, Cp(T) =

$$- 549.25664 + 0.326977T - 3.6189E-04T^2 + 1.145343E-07T^3 - - - - -$$

CHLORINE DIOXIDE ClO₂ 100-1500K

$$Cp(T) = 474.2129 - 0.009513T + 3.445E-03T^2 - 7.92275E-06T^3$$

$$+ 7.90642E-09T^4 - 3.76735E-12T^5 + 6.99282E-16T^6$$

$$Cp(100) = 500.54 \quad Cp(800) = 802.25 \quad Cp(1500) = 855.11$$

- std error est = 1.3 max error est = 2.5 - - - - -

CHLORINE FLUORIDE ClF 250-1500K

$$Cp(T) = 415.24 + 0.88853T - 1.27775E-03T^2 + 9.74189E-07T^3$$

$$- 3.8041674E-10T^4 + 6.015904E-14T^5$$

$$Cp(250) = 571.31 \quad Cp(800) = 670.98 \quad Cp(1500) = 691.96$$

std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, Cp(T) =

$$- 464.27264 + 0.54434T - 4.614077E-04T^2 + 1.3377E-07T^3 - - - - -$$

CHLORINE MONOXIDE Cl₂O 100-1500K

$$\begin{aligned} Cp(T) = & 335.591265 + 0.654343T + 4.97567E-04T^2 - 2.93811E-06T^3 \\ & + 3.65937E-09T^4 - 1.95317E-12T^5 + 3.902384E-16T^6 \\ Cp(100) = & 403.41 \quad Cp(900) = 640.62 \quad Cp(1500) = 659.25 \\ \text{std error est} = & 1.2 \quad \text{max error est} = 2.5 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K, Cp(T) = 329.537164 + 0.83896T - 7.41912E-04T² + 2.20666E-07T³.

CHLORINE OXIDE ClO 100-1500K

$$\begin{aligned} Cp(T) = & 591.2772 - 0.598616T + 4.16749E-03T^2 - 8.65076E-06T^3 \\ & + 8.541837E-09T^4 - 4.10708E-12T^5 + 7.729816E-16T^6 \\ Cp(100) = & 565.25 \quad Cp(900) = 711.69 \quad Cp(1500) = 733.55 \\ \text{std error est} = & 1.5 \quad \text{max error est} = 3.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K, Cp(T) = 515.3754 + 0.426933T - 2.91036E-04T² + 6.836113E-08T³.

CHLORINE TRIFLUORIDE ClF₃ 250-1500K

$$\begin{aligned} Cp(T) = & 80.2859 + 3.96595T - 9.1267E-03T^2 + 1.184492E-05T^3 \\ & - 8.82973E-09T^4 + 3.5203E-12T^5 - 5.80698E-16T^6 \\ Cp(250) = & 655.24 \quad Cp(900) = 868.87 \quad Cp(1500) = 887.998 \\ \text{std error est} = & 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

CHLORODIFLUOROMETHANE CHClF₂ 90-645K

(FREON-22)- Ideal gas

$$\begin{aligned} Cp(T) = & 317.0722 + 0.514191T + 5.95107E-03T^2 - 2.58911E-05T^3 \\ & + 6.22797E-08T^4 - 8.02754E-11T^5 + 4.084E-14T^6 \\ Cp(90) = & 396.31 \quad Cp(400) = 757.51 \quad Cp(645) = 935.32 \\ \text{std error est} = & 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

645-1365K

$$\begin{aligned} Cp(T) = & 276.0442 + 1.6021325T - 1.065933E-03T^2 + 2.585745E-07T^3 \\ Cp(645) = & 935.35 \quad Cp(900) = 1043.06 \quad Cp(1365) = 1134.52 \\ \text{std error est} = & 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

90-645K

$$\begin{aligned} T(Cp) = & 331.0157 - 3.35938Cp + 1.141036E-02Cp^2 - 1.36494E-05Cp^3 \\ & + 6.06808E-09Cp^4 \\ T(396.31) = & 92 \quad T(757.51) = 399 \quad T(935.32) = 646 \\ \text{std error est} = & 1.3 \quad \text{max error est} = 3.5 \end{aligned}$$

645-1365K

$$\begin{aligned} T(Cp) = & 242225.509 - 986.8453Cp + 1.510484Cp^2 - 1.028665E-03Cp^3 \\ & + 2.6358E-07Cp^4 \end{aligned}$$

CHLORODIFLUOROMETHANE (Continued)

$T(935.35) = 644$ $T(1043.06) = 898$ $T(1134.52) = 1365$
 $\underline{\underline{\text{std error est} = 1}}$ $\underline{\underline{\text{max error est} = 1}}$

CHLORODIFLUOROMETHANE, CDCl_2 100-1000K
 MONODEUTERATED

$Cp(T) = 355.67955 - 0.424395T + 1.121936E-02T^2 - 3.137704E-05T^3$
 $+ 4.13097E-08T^4 - 2.71585E-11T^5 + 7.159286E-15T^6$
 $Cp(100) = 397.92$ $Cp(600) = 938.49$ $Cp(1000) = 1084.09$
 $\text{std error est} = 0.6$ $\text{max error est} = 1.0$

$T(Cp) = -2810.61 + 21.0917Cp - 6.179567E-02Cp^2 + 9.22238E-05Cp^3$
 $- 6.82091E-08Cp^4 + 2.022326E-11Cp^5$
 $T(397.92) = 100$ $T(938.49) = 598$ $T(1084.09) = 1000$
 $\underline{\underline{\text{std error est} = 1.3}}$ $\underline{\underline{\text{max error est} = 2.5}}$

CHLOROFORM - Ideal gas CHCl_3 100-755K

$Cp(T) = 189.1583 + 1.598713T - 1.340133E-03T^2 + 5.419056E-09T^3$
 $+ 3.77955E-10T^4$
 $Cp(100) = 335.67$ $Cp(500) = 677.78$ $Cp(755) = 757.42$
 $\text{std error est} = 0.2$ $\text{max error est} = 1.0$

$T(Cp) = 402.7039 + 0.7755899T - 4.920244E-04T^2 + 1.152399E-07T^3$
 $Cp(755) = 757.40$ $Cp(1000) = 801.51$ $Cp(1365) = 837.72$
 $\text{std error est} = 0.2$ $\text{max error est} = 1.0$

$T(Cp) = 1673.1583 - 14.61295Cp + 4.77988E-02Cp^2 - 6.568945E-05Cp^3$
 $+ 3.424226E-08Cp^4$
 $T(335.67) = 104$ $T(677.78) = 500$ $T(757.42) = 753$
 $\text{std error est} = 1.8$ $\text{max error est} = 3.5$

$T(Cp) = -179838.72 + 710.17532Cp - 0.936808Cp^2 + 4.14539E-04Cp^3$
 $T(757.40) = 755$ $T(801.51) = 1000$ $T(837.72) = 1365$
 $\underline{\underline{\text{std error est} = 0.8}}$ $\underline{\underline{\text{max error est} = 2.5}}$

CHLOROFUOROMETHANE CH_2ClF 200-1000K

$Cp(T) = 638.4166 - 2.34596T + 1.549633E-02T^2 - 3.2233E-05T^3$
 $+ 3.40267E-08T^4 - 1.8304265E-11T^5 + 3.978875E-15T^6$
 $Cp(200) = 580.05$ $Cp(600) = 1019.35$ $Cp(1000) = 1257.1$
 $\text{std error est} = 0.4$ $\text{max error est} = 1.0$

$T(Cp) = -1079.2262 + 4.074Cp - 4.3312E-03Cp^2 + 1.912603E-06Cp^3$
 $T(580.05) = 200$ $T(1019.35) = 599$ $T(1257.1) = 997$
 $\underline{\underline{\text{std error est} = 1.4}}$ $\underline{\underline{\text{max error est} = 3}}$

CHLOROMETHYLIDYNE CC1 300-1500K

$$\begin{aligned} \text{Cp}(T) = & 543.19413 + 0.651587T - 7.2857E-04T^2 + 3.84102E-07T^3 \\ & - 7.77988E-11T^4 \end{aligned}$$

$$\begin{aligned} \text{Cp}(300) = & 682.84 & \text{Cp}(800) = 762.97 & \text{Cp}(1500) = 783.78 \\ \text{std error est} = & 0.4 & & \text{max error est} = 1.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1500K, Cp(T) = $570.92334 + 0.48166T - 3.8583E-04T^2 + 1.066284E-07T^3$ -----

CHLOROSILANE SiH₃Cl 100-1000K

$$\begin{aligned} \text{Cp}(T) = & 632.108 - 3.352308T + 2.6872E-02T^2 - 7.054946E-05T^3 \\ & + 9.37112E-08T^4 - 6.27597E-11T^5 + 1.67893E-14T^6 \\ \text{Cp}(100) = & 503.81 & \text{Cp}(500) = 1013.31 & \text{Cp}(1000) = 1343.14 \\ \text{std error est} = & 1.6 & & \text{max error est} = 3.0 \end{aligned}$$

CHLOROTRIFLUOROMETHANE CC1F₃ 200-1090K

(FREON-13) - Ideal gas

$$\begin{aligned} \text{Cp}(T) = & 77.23115 + 2.79399T - 3.680032E-03T^2 + 2.4349E-06T^3 \\ & - 6.56569E-10T^4 \\ \text{Cp}(200) = & 507.26 & \text{Cp}(600) = 869.66 & \text{Cp}(1090) = 976.9 \\ \text{std error est} = & 0.3 & & \text{max error est} = 1.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 200-1090, Cp(T) = $137.21148 + 2.290486T - 2.25364E-03T^2 + 7.92858E-07T^3$ -----

CUMENE C₆H₅CH(CH₃)₂ 275-1500K

$$\begin{aligned} \text{Cp}(T) = & 80.85313 + 2.55483T + 1.017634E-02T^2 - 2.428585E-05T^3 \\ & + 2.32E-08T^4 - 1.05785E-11T^5 + 1.8904E-15T^6 \\ \text{Cp}(275) = & 1164.81 & \text{Cp}(800) = 2735.13 & \text{Cp}(1500) = 3497.47 \\ \text{std error est} = & 1.7 & & \text{max error est} = 5 \end{aligned}$$

275-1500K

$$\begin{aligned} \text{T(Cp)} = & 622.8356 - 1.098344\text{Cp} + 1.04225E-03\text{Cp}^2 - 3.612275E-07\text{Cp}^3 \\ & + 4.95368E-11\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} \text{T(1164.81)} = & 278 & \text{T(2735.13)} = 797 & \text{T(3497.47)} = 1489 \\ \text{std error est} = & 4.0 & & \text{max error est} = 14 \end{aligned}$$

CYANOGEN (CN)₂ 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 311.4587 + 4.93727T - 1.16917E-02T^2 + 1.6521E-05T^3 \\ & - 1.31327E-08T^4 + 5.4334E-12T^5 - 9.1145E-16T^6 \\ \text{Cp}(100) = & 703.53 & \text{Cp}(800) = 1399.67 & \text{Cp}(1500) = 1563.02 \\ \text{std error est} = & 1.2 & & \text{max error est} = 2.5 \end{aligned}$$

CYANOGEN CHLORIDE CNC1 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 287.6997 + 2.740703T - 6.197496E-03T^2 + 8.19973E-06T^3 \\ & - 6.1265E-09T^4 + 2.39758E-12T^5 - 3.82468E-16T^6 \end{aligned}$$

$$\text{Cp}(100) = 507.41 \quad \text{Cp}(800) = 888.09 \quad \text{Cp}(1500) = 963.14$$

- std error est = 1.1 - max error est = 2.5

CYCLOHEXANE - See HEXANE

CYCLOPROPANE - See PROPANE

n-DECANE - Ideal gas C₁₀H₂₂ 300-700K

$$\begin{aligned} \text{Cp}(T) = & 240.7178 + 5.09965T - 6.29026E-04T^2 - 1.07155E-06T^3 \\ \text{Cp}(300) = & 1685.07 \quad \text{Cp}(500) = 2499.34 \quad \text{Cp}(700) = 3134.71 \\ \text{std error est} = & 0.1 \quad \text{max error est} = 1.0 \end{aligned}$$

700-1365K

$$\begin{aligned} \text{Cp}(T) = & -13534.589 + 91.4879T - 0.2207T^2 + 2.91406E-04T^3 \\ & - 2.153074E-07T^4 + 8.386E-11T^5 - 1.34404E-14T^6 \end{aligned}$$

$$\begin{aligned} \text{Cp}(700) = & 3134.09 \quad \text{Cp}(1000) = 3771.91 \quad \text{Cp}(1365) = 4258.15 \\ \text{std error est} = & 1.2 \quad \text{max error est} = 2.0 \end{aligned}$$

300-700K

$$\begin{aligned} \text{T(Cp)} = & -201.2556 + 0.4224556\text{Cp} - 1.10665E-04\text{Cp}^2 + 2.15458E-08\text{Cp}^3 \\ \text{T}(1685.07) = & 299 \quad \text{T}(2499.34) \approx 500 \quad \text{T}(3134.71) = 699 \\ \text{std error est} = & 0.3 \quad \text{max error est} = 1 \end{aligned}$$

700-1365K

$$\begin{aligned} \text{T(Cp)} = & 11052.013 - 13.05146\text{Cp} + 5.9256E-03\text{Cp}^2 - 1.1798E-06\text{Cp}^3 \\ & + 8.983E-11\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} \text{T}(3134.09) = & 699 \quad \text{T}(3771.91) \approx 998 \quad \text{T}(4258.15) = 1362 \\ \text{std error est} = & 0.5 \quad \text{max error est} = 3 \end{aligned}$$

n-DEUTERIUM D₂ 200-645K

Ideal gas

$$\begin{aligned} \text{Cp}(T) = & 7264.2197 + 0.037477T - 7.05335E-04T^2 + 1.51166E-06T^3 \\ \text{Cp}(200) = & 7255.6 \quad \text{Cp}(400) = 7264.28 \quad \text{Cp}(645) = 7400.59 \\ \text{std error est} = & 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

645-1365K

$$\begin{aligned} \text{Cp}(T) = & 7583.3708 - 2.017012T + 3.3723E-03T^2 - 1.080913E-06T^3 \\ \text{Cp}(645) = & 7395.31 \quad \text{Cp}(1000) = 7857.75 \quad \text{Cp}(1365) = 6364.41 \\ \text{std error est} = & 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqns: 200-645K, Cp(T) = 7353.022 - 0.72328T + 1.2086E-03T²; 645-1365K, Cp(T) = 6629.115 + 1.06105T + 1.642087E-04T².

DEUTERIUM (Monatomic) D 55-1500K

- Cp(T) = 10.32 - constant - - - - -

DIBROMOMETHANE CH_2Br_2 300-1000K

$\text{Cp}(T) = 104.624 + 0.911614T - 7.67807E-04T^2 + 2.58695E-07T^3$
 $\text{Cp}(300) = 315.99 \quad \text{Cp}(600) = 431.06 \quad \text{Cp}(1000) = 507.13$
std error est = 0.3 max error est = 1.0

300-1000K
 $T(\text{Cp}) = -2029.747 + 17.57971\text{Cp} - 4.78704E-02\text{Cp}^2 + 4.927377E-05\text{Cp}^3$
 $T(315.99) = 300 \quad T(431.06) = 600 \quad T(507.13) = 1001$

- std error est = 0.7 - - - - - max error est = 1.5

DICHLORODIFLUOROMETHANE 100-1365K CCl_2F_2

(FREON-12) - Ideal gas

$\text{Cp}(T) = 115.7338 + 2.37887T - 2.812186E-03T^2 + 5.571888E-07T^3$
+ $1.82207E-09T^4 - 1.6317E-12T^5 + 4.2395E-16T^6$
 $\text{Cp}(100) = 326.22 \quad \text{Cp}(800) = 827.04 \quad \text{Cp}(1365) = 875.74$

- std error est = 0.3 - - - - - max error est = 1.0

1,1-DICHLORO-1-FLUORO-300-600K CH_3CFCl_2
ETHANE

$\text{Cp}(T) = 474 + 1.0T \quad T(\text{Cp}) = \text{Cp} - 474$

Note: There are only three (3) data points available from the
- reference source. The accuracy cannot be adequately established.

DICHLOROFUOROMETHANE 100-755K CHCl_2F

(FREON-21) - Ideal gas

$\text{Cp}(T) = 209.72 + 1.79069T - 3.45786E-03T^2 + 1.0810155E-05T^3$
- $2.22979E-08T^4 + 2.16214E-11T^5 - 7.79904E-15T^6$
 $\text{Cp}(100) = 362.999 \quad \text{Cp}(450) = 720.25 \quad \text{Cp}(755) = 857.42$

std error est = 0.3 max error est = 1.0

755-1365K

$\text{Cp}(T) = 388.2867 + 1.023759T - 6.4682E-04T^2 + 1.50429E-07T^3$
 $\text{Cp}(755) = 857.26 \quad \text{Cp}(1000) = 915.65 \quad \text{Cp}(1365) = 963.13$
std error est = 0.2 max error est = 1.0

100-755K

$T(\text{Cp}) = 921.3768 - 7.7154\text{Cp} + 2.414285E-02\text{Cp}^2 - 3.033265E-05\text{Cp}^3$
+ $1.446893E-08\text{Cp}^4$

$T(362.99) = 102 \quad T(720.25) = 449 \quad T(857.42) = 755$
std error est = 1.1 max error est = 2.0

755-1365K

$T(\text{Cp}) = -122177 + 424.7354\text{Cp} - 0.493077\text{Cp}^2 + 1.923554E-04\text{Cp}^3$
 $T(857.26) = 755 \quad T(915.65) = 999 \quad T(963.13) = 1364$
std error est = 1.1 max error est = 2.0

DICHLOROFLUOROMETHANE, 100-1000K CDCl_2F
 MONODEUTERATED
 $\text{Cp}(\text{T}) = 255.720254 + 0.689369\text{T} + 4.583258\text{E}-03\text{T}^2 - 1.3455115\text{E}-05\text{T}^3$
 $+ 1.377348\text{E}-08\text{T}^4 - 4.9189282\text{E}-12\text{T}^5$
 $\text{Cp}(100) = 358.36 \quad \text{Cp}(500) = 771.46 \quad \text{Cp}(1000) = 927.78$
 $\underline{\text{std error est}} = 5.8 \quad \underline{\text{max error est}} = 10$
DICHLOROMETHANE CH_2Cl_2 275-1500K
 $\text{Cp}(\text{T}) = 132.0712 + 2.141377\text{T} - 2.08642\text{E}-03\text{T}^2 + 1.059563\text{E}-06\text{T}^3$
 $- 2.15869\text{E}-10\text{T}^4$
 $\text{Cp}(275) = 583.97 \quad \text{Cp}(800) = 963.94 \quad \text{Cp}(1500) = 1132.88$
 $\underline{\text{std error est}} = 0.9 \quad \underline{\text{max error est}} = 2.0$
275-1500K
 $\text{T}(\text{Cp}) = 5523.4 - 29.33479\text{Cp} + 5.93745\text{E}-02\text{Cp}^2 - 5.22736\text{E}-05\text{Cp}^3$
 $+ 1.760695\text{E}-08\text{Cp}^4$
 $\text{T}(583.97) = 278 \quad \text{T}(963.94) = 797 \quad \text{T}(1132.88) = 1491$
 $\underline{\text{std error est}} = 5.0 \quad \underline{\text{max error est}} = 9$
1,1-DICHLOROTETRAFLUORO- 275-600K CCl_2FCF_3
ETHANE
 $\text{Cp}(\text{T}) = -104.2484 + 4.520335\text{T} - 8.19256\text{E}-03\text{T}^2 + 5.7332\text{E}-06\text{T}^3$
 $\text{Cp}(275) = 638.51 \quad \text{Cp}(450) = 793.35 \quad \text{Cp}(600) = 897.00$
 $\underline{\text{std error est}} = 0.01 \quad \underline{\text{max error est}} = 0.5$
275-600K
 $\text{T}(\text{Cp}) = 421.358 - 1.292708\text{Cp} + 1.66326\text{E}-03\text{Cp}^2$
 $\text{T}(638.51) = 274 \quad \text{T}(793.35) = 443 \quad \text{T}(897.00) = 600$
 $\underline{\text{std error est}} = 1.4 \quad \underline{\text{max error est}} = 2.5$
DICHLOROTETRAFLUORO- 220-510K $\text{C}_2\text{Cl}_2\text{F}_4$
ETHANE (FREON-114)
 $\text{Cp}(\text{T}) = -94.71864 + 4.57011\text{T} - 7.699598\text{E}-03\text{T}^2 + 4.89705\text{E}-06\text{T}^3$
 $\text{Cp}(220) = 590.19 \quad \text{Cp}(400) = 814.8 \quad \text{Cp}(510) = 882.97$
 $\underline{\text{std error est}} = 0.2 \quad \underline{\text{max error est}} = 1.0$
220-510K
 $\text{T}(\text{Cp}) = -1652.37 + 7.94254\text{Cp} - 1.184297\text{E}-02\text{Cp}^2 + 6.36623\text{E}-06\text{Cp}^3$
 $\text{T}(590.19) = 219 \quad \text{T}(814.8) = 400 \quad \text{T}(882.97) = 510$
 $\underline{\text{std error est}} = 0.5 \quad \underline{\text{max error est}} = 1.5$
2,2-DICHLORO-1,1,1-TRI- 200-800K F_3CCHCl_2
FLUOROETHANE
 $\text{Cp}(\text{T}) = 1319.2995 - 14.01811\text{T} + 8.407976\text{E}-02\text{T}^2 - 2.15252\text{E}-04\text{T}^3$
 $+ 2.57008\text{E}-07\text{T}^4 - 1.15831\text{E}-10\text{T}^5$
 $\text{Cp}(200) = 530.999 \quad \text{Cp}(500) = 866.97 \quad \text{Cp}(800) = 1021.81$
 $\underline{\text{std error est}} = 0.5 \quad \underline{\text{max error est}} = 2.5*$
~~*Note: $\text{Cp}(700) = 1114.17$ but table value is 984.~~

1,1-DIFLUOROETHYLENE CH₂CF₂ 175-1175K

Cp(T) = 472.82 - 1.09967T + 1.798667E-02T² - 4.64504E-05T³
+ 5.802696E-08T⁴ - 3.622937E-11T⁵ + 8.981685E-15T⁶
Cp(175) = 631.01 Cp(600) = 1377.09 Cp(1175) = 1760.59
std error est = 4.4 max error est = 8
DIFLUOROMETHANE CH₂F₂ 200-1000K

Cp(T) = 926.6998 - 4.228109T + 2.28603E-02T² - 4.39433E-05T³
+ 4.39172E-08T⁴ - 2.27523E-11T⁵ + 4.84046E-15T⁶
Cp(200) = 707.24 Cp(500) = 1144.26 Cp(1000) = 1620.95
std error est = 0.5 max error est = 1.0
200-1000K
T(Cp) = -1024.354 + 3.046388Cp - 2.430315E-03Cp² + 8.15023E-07Cp³
T(707.24) = 203 T(1144.26) = 500 T(1620.95) = 999
std error est = 1.5 max error est = 3.5
DIMETHYLAMINE (CH₃)₂NH 275-1475K

Cp(T) = 843.8386 - 1.419 1273T + 2.18139E-02T² - 4.059054E-05T³
+ 3.603484E-08T⁴ - 1.5961557E-11T⁵ + 2.82084E-15T⁶
Cp(275) = 1441.30 Cp(800) = 3156.13 Cp(1475) = 4128.28
std error est = 2.4 max error est = 4.5
275-1475K
T(Cp) = 389.02765 - 0.587004715Cp + 5.4705492E-04Cp² - 1.6211353E-07Cp³
+ 1.92366E-11Cp⁴
T(1441.30) = 277 T(3156.13) = 798 T(4128.28) = 1471
std error est = 3.5 max error est = 6
2,2-DIMETHYLBUTANE CH₃CH₂C(CH₃)₃ 300-1000K

Cp(T) = 2581.4188 - 21.863667T + 0.11908912T² - 2.667096E-04T³
+ 3.179459E-07T⁴ - 1.9721679E-10T⁵ + 5.005353E-14T⁶
Cp(300) = 1671.79 Cp(600) = 2931.54 Cp(1000) = 3879.91
std error est = 1.8 max error est = 2.5
300-1000K
T(Cp) = -245.69753 + 0.521407Cp - 1.6592016E-04Cp² + 2.9471092E-08Cp³
T(1671.79) = 300 T(2931.54) = 599 T(3879.91) = 1001
std error est = 1.6 max error est = 2.5
2,3-DIMETHYLBUTANE [(CH₃)₂CH]₂ 300-1000K

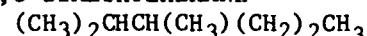
Cp(T) = 734.10753 - 0.560625T + 2.23453E-02T² - 4.17216E-05T³
+ 3.25804E-08T⁴ - 9.52277E-12T⁵
Cp(300) = 1691.27 Cp(600) = 2912.1 Cp(1000) = 3854.81
std error est = 2.2 max error est = 4.5

2, 3-DIMETHYLBUTANE (Continued) 300-1000K

$$T(Cp) = -218.0723 + 0.473152Cp - 1.438724E-04Cp^2 + 2.6738645E-08Cp^3$$

$$T(1691.27) = 300 \quad T(2912.1) = 600 \quad T(3854.81) = 1000$$

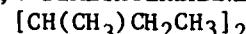
std error est = 0.7 max error est = 1.5

2, 3-DIMETHYLHEXANE 395-520K

$$Cp(T) = 605.9 + 3.8822T \quad T(Cp) = [Cp - 605.9]/3.8822$$

Note: There are only three data points in the reference source.

The accuracy of the fits cannot be adequately estimated.

3, 4-DIMETHYLHEXANE 405-520K

$$Cp(T) = 594.01 + 3.881T \quad T(Cp) = [Cp - 594.01]/3.881$$

Note: There are only three data points in the reference source.

The accuracy of the fits cannot be adequately estimated.

DIMETHYLPROPANE $C(CH_3)_4$ 300-1500K

$$\ln[Cp(T)] = 6.1724277 + 5.9032424E-03T - 6.648126E-06T^2 \\ + 3.6018484E-09T^3 - 7.508868E-13T^4$$

$$**Cp(T) = \exp[fctn(T)]$$

$$Cp(300) = 1696.35 \quad Cp(800) = 3557.47 \quad Cp(1500) = 4554.55$$

std error est = 8.00674E-03 for $\ln[Cp(T)]$

DIPROPYLENE GLYCOL $(CH_3CHOHCH_2)_2O$ 275-775K

$$Cp(T) = -1826.75484 + 36.04835T - 0.1900801T^2 + 5.610031E-04T^3 \\ - 9.03165E-07T^4 + 7.46426E-10T^5 - 2.482783E-13T^6$$

$$Cp(275) = 1280.09 \quad Cp(500) = 1801.43 \quad Cp(775) = 2155.97$$

std error est = 2.8 max error est = 3.5

$$T(Cp) = -395.8809 + 0.389689Cp + \frac{275-775K}{5.172082E-04Cp^2 - 4.901004E-07Cp^3} \\ + 1.31177E-10Cp^4$$

$$T(1280.09) = 275 \quad T(1801.43) = 501 \quad T(2155.97) = 771$$

std error est = 2.4 max error est = 5

DODECANE $CH_3(CH_2)^{10}CH_3$ 300-1500K

$$Cp(T) = 827.74543 - 0.177414T + 1.89547E-02T^2 - 3.681404E-05T^3 \\ + 3.299875E-08T^4 - 1.45863E-11T^5 + 2.55543E-15T^6$$

$$Cp(300) = 1720.17 \quad Cp(800) = 3374.57 \quad Cp(1500) = 4361.72$$

std error est = 5.0 max error est = 7.5

$$T(Cp) = 867.5699 - 1.28664Cp + \frac{300-1500K}{8.801372E-04Cp^2 - 2.28373E-07Cp^3} \\ + 2.333242E-11Cp^4$$

$$T(1720.17) = 301 \quad T(3374.57) = 798 \quad T(4361.72) = 1496$$

std error est = 4.5 max error est = 7.5

ETHANE - Ideal gas C₂H₆ 275-755K

$C_p(T) = 531.9795 + 3.755877T + 1.789289E-03T^2 - 2.13225E-06T^3$
 $C_p(275) = 1655.82 \quad C_p(500) = 2590.71 \quad C_p(755) = 3469.95$
 std error est = 0.1 max error est = 1.0

755-1365K

$$Cp(T) = 3718.3729 - 10.891558T + 2.95115E-02T^2 - 2.95597E-05T^3$$

$$+ 1.382794E-08T^4 - 2.52553E-12T^5$$

$$Cp(755) = 3469.49 \quad Cp(1000) = 4081.02 \quad Cp(1365) = 4696.05$$

$$\text{std error est} = 0.4 \quad \text{max error est} = 1.0$$

$T(Cp) = 26.69485 - 0.0209973Cp + 1.77038E-04Cp^2 - 5.60605E-08Cp^3$
 $+ 6.976759E-12Cp^4$
 $T(1655.82) = 275 \quad T(2590.71) = 500 \quad T(3469.95) = 755$
 std error est = 0.2 max error est = 1

$$\begin{aligned} & \text{755-1365K} \\ T(Cp) &= -3405.9176 + 2.9438457Cp - 7.63789E-04Cp^2 + 7.521499E-08Cp^3 \\ T(3469.49) &= 755 \quad T(4081.02) = 1000 \quad T(4696.05) = 1364 \\ \underline{\text{std error est}} &= 0.5 \quad \underline{\text{max error est}} = 1.5 \end{aligned}$$

ETHANE , HEXADEUTERATED C₂D₆ 275-365K

$C_p(T) = 1100.6747 - 3.438783T + 2.9385375E-02T^2 - 3.3966273E-05T^3$
 $C_p(275) = 1670.89 \quad C_p(315) = 1871.58 \quad C_p(365) = 2108.7$
 std error est = 0.1 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the polynomial above.

ETHANETHIOL C₂H₅SH 300-1000K

$C_p(T) = 357.285 + 2.59852T + 1.61883E-03T^2 - 4.13005E-06T^3$
 $+ 1.930025E-09T^4$
 $C_p(300) = 1186.66 \quad C_p(700) = 2016.27 \quad C_p(1000) = 2374.61$
 $\text{std error est} = 5.5 \quad \text{max error est} = 9.5$
 $T(C_p) = -340.822 + 0.8964337C_p - 4.606323E-04C_p^2 + 1.352216E-07C_p^3$
 $T(1186.66) = 300 \quad T(2016.27) = 702 \quad T(2374.61) = 1001$
 $\text{std error est} = 4.8 \quad \text{max error est} = 6.5$

ETHYL ACETATE CH₃COOCH₂CH₃ 370-440K

$Cp(T) = -1312.0132 + 11.8064T - 1.1402197E-02T^2$
 $Cp(370) = 1495.39 \quad Cp(400) = 1586.2 \quad Cp(440) = 1675.34$
 std error est = 8.3 max error est = 15

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the equation above. The T(Cp) calculations may not agree well due to the std error ests above.

ETHYL ALCOHOL C₂H₅OH 255-810K
 Ideal gas
 $C_p(T) = 546.2212 + 3.8600396T - 1.023837E-03T^2 - 2.75659E-07T^3$
 $C_p(255) = 1459.39 \quad C_p(500) = 2185.82 \quad C_p(810) = 2854.62$
 $\text{std error est} = 0.3 \quad \text{max error est} = 1.5$

$$\frac{810-1365K}{C_p(T) = 835.49557 + 3.1089285T - 4.372953E-04T^2 - 5.607147E-07T^3 + 2.0162334E-10T^4}$$

 $C_p(810) = 2855.62 \quad C_p(1100) = 3275.08 \quad C_p(1365) = 3538.29$
 $\text{std error est} = 0.2 \quad \text{max error est} = 1.0$

$$\frac{255-810K}{T(C_p) = -394.5867 + 0.668288C_p - 2.236847E-04C_p^2 + 4.805682E-08C_p^3}$$

 $T(1459.39) = 254 \quad T(2185.82) = 499 \quad T(2854.62) = 808$
 $\text{std error est} = 0.7 \quad \text{max error est} = 2$

$$\frac{810-1365K}{T(C_p) = -7130.17 + 7.512807C_p - 2.545385E-03C_p^2 + 3.11057E-07C_p^3}$$

 $T(2855.62) = 810 \quad T(3275.08) = 1100 \quad T(3538.29) = 1364$
 $\text{std error est} = 0.2 \quad \text{max error est} = 2$
ETHYLBENZENE C₆H₅C₂H₅ 275-1500K
 $C_p(T) = 88.81893 + 2.2813924T + 1.0434866E-02T^2 - 2.431028E-05T^3 + 2.3069044E-08T^4 - 1.0491076E-11T^5 + 1.87293E-15T^6$
 $C_p(275) = 1116.01 \quad C_p(800) = 2647.73 \quad C_p(1500) = 3396.43$
 $\text{std error est} = 1.9 \quad \text{max error est} = 6$

$$\frac{275-1500K}{T(C_p) = 642.15192 - 1.1750234C_p + 1.1452373E-03C_p^2 - 4.0876E-07C_p^3 + 5.746896E-11C_p^4}$$

 $T(1116.01) = 278 \quad T(2647.73) = 797 \quad T(3396.43) = 1495$
 $\text{std error est} = 3.9 \quad \text{max error est} = 8$
ETHYL ETHER C₄H₁₀O 310-600K
 $C_p(T) = -4053.47326 + 33.471276T - 6.7641844E-02T^2 + 5.094208E-05T^3$
 $C_p(310) = 1339.87 \quad C_p(450) = 1953.22 \quad C_p(600) = 2681.72$
 $\text{std error est} = 0.2 \quad \text{max error est} = 1.0$

$$\frac{310-600K}{T(C_p) = 779.23434 - 1.052998C_p + 6.81429E-04C_p^2 - 1.17146E-07C_p^3}$$

 $T(1339.87) = 310 \quad T(1953.22) = 449 \quad T(2681.72) = 597$
 $\text{std error est} = 1.5 \quad \text{max error est} = 3$
ETHYLENE - Ideal gas C₂H₄ 275-755K
 $C_p(T) = 248.817245 + 4.864076T - 1.570483E-03T^2 - 2.3772E-07T^3$
 $C_p(275) = 1462.73 \quad C_p(500) = 2258.52 \quad C_p(755) = 2923.67$
 $\text{std error est} = 0.2 \quad \text{max error est} = 1.0$

ETHYLENE - Ideal gas (continued) 755-1365K

$$C_p(T) = 883.873 + 2.982773T + 2.684874E-04T^2 - 1.103103E-06T^3 + 3.3579064E-10T^4$$

$$C_p(755) = 2923.28 \quad C_p(1000) = 3367.82 \quad C_p(1365) = 3815.82 \\ \text{std error est} = 0.3 \quad \text{max error est} = 1.0$$

$$\frac{275-755K}{T(C_p) = -215.2115 + 0.46972C_p - 1.376816E-04C_p^2 + 3.0917277E-08C_p^3} \\ T(1462.73) = 274 \quad T(2258.52) = 500 \quad T(2923.67) = 754 \\ \text{std error est} = 0.5 \quad \text{max error est} = 2$$

$$\frac{755-1365K}{T(C_p) = -4851.525 + 4.91917C_p - 1.56526E-03C_p^2 + 1.842345E-07C_p^3} \\ T(2923.28) = 755 \quad T(3367.82) = 999 \quad T(3815.82) = 1364 \\ \text{std error est} = 0.5 \quad \text{max error est} = 1$$

ETHYLENE - Real gas 275-610K

$$C_p(T) = 452.40453 + 3.594527T + 1.099394E-03T^2 - 2.103391E-06T^3 \\ C_p(275) = 1480.3 \quad C_p(450) = 2100.9 \quad C_p(610) = 2576.72 \\ \text{std error est} = 1.5 \quad \text{max error est} = 2.5$$

Note: For $T(C_p)$ calculations, use the iterative procedures discussed in Section 5 and the polynomial immediately above.

ETHYLENE OXIDE $(CH_2)_2O$ 275-1000K

$$C_p(T) = 1405.23696 - 8.747353T + 4.235163E-02T^2 - 6.972269E-05T^3 + 5.2382475E-08T^4 - 1.5060405E-11T^5 \\ C_p(275) = 1028.44 \quad C_p(600) = 1960.98 \quad C_p(1000) = 2608.89 \\ \text{std error est} = 5.0 \quad \text{max error est} = 7.5$$

$$\frac{275-1365K}{T(C_p) = -324.12166 + 0.929479C_p - 4.506574E-04C_p^2 + 1.107183E-07C_p^3} \\ T(1028.44) = 276 \quad T(1960.98) = 600 \quad T(2608.89) = 999 \\ \text{std error est} = 1.5 \quad \text{max error est} = 3$$

3-ETHYLHEXANE $(CH_3CH_2)_2CH(CH_2)_2CH_3$ 295-520K

$$C_p(T) = 1559.9 + 1.928T \quad T(C_p) = [C_p - 1559.9]/1.928$$

Note: There are only three data points in the reference source.

The accuracy of the fit cannot be adequately established.

3-ETHYL-2-METHYL- $(CH_3)_2CHCH(C_2H_5)_2$ 400-520K
PENTANE

$$C_p(T) = 658.8 + 3.7806T \quad T(C_p) = [C_p - 658.8]/3.7806$$

Note: There are only three data points in the reference source.

The accuracy of the fit cannot be adequately established.

3-ETHYL-3-METHYL- $(CH_3CH_2)_3CCH_3$ 400-520K
PENTANE

$$C_p(T) = 641.9 + 3.8767T \quad T(C_p) = [C_p - 641.9]/3.8767$$

Note: There are only three data points in the reference source.

The accuracy of the fit cannot be adequately established.

FLUORINE F₂ 200-645K
 Ideal gas
 $C_p(T) = 658.25722 + 0.6751476T - 3.79745E-04T^2 + 2.235484E-09T^3$
 $C_p(200) = 778.11 \quad C_p(450) = 885.38 \quad C_p(645) = 936.34$
 $\text{std error est} = 0.01 \quad \text{max error est} = 1.0$
645-1365K
 $C_p(T) = 127.23948 + 3.72368T - 7.033226E-03T^2 + 6.867834E-06T^3$
 $- 3.366543E-09T^4 + 6.5637923E-13T^5$
 $C_p(645) = 936.51 \quad C_p(1000) = 975.36 \quad C_p(1365) = 995.65$
 $\text{std error est} = 0.3 \quad \text{max error est} = 1.0$
200-645K
 $T(C_p) = 3954.34 - 11.05956C_p + 8.024798E-03C_p^2$
 $T(778.11) = 207 \quad T(885.38) = 453 \quad T(936.34) = 634$
 $\text{std error est} = 5.0 \quad \text{max error est} = 11$
645-1365K
 $T(C_p) = 112357.756 - 242.565496C_p + 0.131647C_p^2$
 $T(936.51) = 654 \quad T(975.36) = 1008 \quad T(995.65) = 1351$
 $\text{std error est} = 7.5 \quad \text{max error est} = 15.5$

FLUORINE (Monatomic) F 100-1500K

$C_p(T) = 925.04634 + 2.7925687T - 1.038958E-02T^2 + 1.78943E-05T^3$
 $- 1.6070342E-08T^4 + 7.28505E-12T^5 - 1.315903E-15T^6$
 $C_p(100) = 1116.77 \quad C_p(800) = 1131.45 \quad C_p(1500) = 1106.39$
 $\text{std error est} = 1.7 \quad \text{max error est} = 3.5$

FLUOROETHANE CH₃CH₂F 100-1500K

$\ln[C_p(T)] = 6.471145519 + 2.09924177E-03T + 1.99348096E-06T^2$
 $- 5.55076164E-09T^3 + 3.8054008E-12T^4 - 8.6180454E-16T^5$
 $C_p(100) = 809.02 \quad C_p(800) = 2593.26 \quad C_p(1500) = 3268.33$
 $\text{std error est} = 10.0 \quad \text{max error est} = 85$
 **Note: $C_p(T) = \exp[fctn(T)]$

FLUOROETHYLENE CH₂CHF 175-975K

$C_p(T) = 580.68945 - 1.7973376T + 2.027156E-02T^2 - 4.167712E-05T^3$
 $+ 3.705407E-08T^4 - 1.2304487E-11T^5$
 $C_p(175) = 696.34 \quad C_p(600) = 1643.20 \quad C_p(975) = 2113.99$
 $\text{std error est} = 7.1 \quad \text{max error est} = 13.5$
175-975K
 $T(C_p) = -171.8982 + 0.671097C_p - 3.337414E-04C_p^2 + 1.285454E-07C_p^3$
 $T(696.34) = 177 \quad T(1643.20) = 600 \quad T(2113.99) = 970$
 $\text{std error est} = 5.5 \quad \text{max error est} = 10$

FLUOROFORM, MONODEUTERATED CF_3D 100-1000K

$$\begin{aligned} \text{Cp}(T) = & 529.7845 - 1.9731807T + 1.8510456E-02T^2 - 4.45372E-05T^3 \\ & + 5.268778E-08T^4 - 3.146596E-11T^5 + 7.57734E-15T^6 \end{aligned}$$

$$\begin{aligned} \text{Cp}(100) = & 477.99 & \text{Cp}(600) = & 1124.68 & \text{Cp}(1000) = & 1329.02 \\ \text{std error est} = & 0.6 & & & & \text{max error est} = 1.0 \end{aligned}$$

100-1000K

$$\begin{aligned} T(\text{Cp}) = & -134.042 - 0.440011\text{Cp} + 3.65192E-03\text{Cp}^2 - 4.4091204E-06\text{Cp}^3 \\ & + 1.799033E-09\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} T(477.99) = & 102 & T(1124.68) = & 596 & T(1329.02) = & 994 \\ \text{std error est} = & 5.8 & & & & \text{max error est} = 10 \end{aligned}$$

FLUOROMETHANE CH_3F 200-1000K

$$\begin{aligned} \text{Cp}(T) = & 1472.3652 - 6.384875T + 0.0269437T^2 - 4.020256E-05T^3 \\ & + 2.816384E-08T^4 - 7.7050064E-12T^5 \end{aligned}$$

$$\begin{aligned} \text{Cp}(200) = & 994.09 & \text{Cp}(600) = & 1708.08 & \text{Cp}(1000) = & 2289.27 \\ \text{std error est} = & 0.8 & & & & \text{max error est} = 2.5 \end{aligned}$$

200-1000K

$$\begin{aligned} T(\text{Cp}) = & -2770.3792 + 6.5625134\text{Cp} - 5.26989E-03\text{Cp}^2 + 1.946297E-06\text{Cp}^3 \\ & - 2.543208E-10\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} T(994.09) = & 209 & T(1708.08) = & 598 & T(2289.27) = & 1000 \\ \text{std error est} = & 4.7 & & & & \text{max error est} = 9.5 \end{aligned}$$

FORMALDEHYDE HCHO 275-1500K

$$\begin{aligned} \text{Cp}(T) = & 1410.7255 - 3.85954T + 1.56866E-02T^2 - 2.25445E-05T^3 \\ & + 1.689E-08T^4 - 6.5741125E-12T^5 + 1.049515E-15T^6 \end{aligned}$$

$$\begin{aligned} \text{Cp}(275) = & 1153.51 & \text{Cp}(800) = & 1858.8 & \text{Cp}(1500) = & 2366.67 \\ \text{std error est} = & 2.0 & & & & \text{max error est} = 4.5 \end{aligned}$$

275-1500K

$$\begin{aligned} T(\text{Cp}) = & -302.25 - 0.79339952\text{Cp} + 2.386302E-03\text{Cp}^2 - 1.438642E-06\text{Cp}^3 \\ & + 2.990445E-10\text{Cp}^4 \end{aligned}$$

$$\begin{aligned} T(1153.51) = & 279 & T(1858.8) = & 798 & T(2366.67) = & 1497 \\ \text{std error est} = & 3.9 & & & & \text{max error est} = 7 \end{aligned}$$

FORMYL HCO 300-1000K

$$\text{Cp}(T) = 978.65 + 0.6283T \quad T(\text{Cp}) = [\text{Cp} - 978.65]/0.6283$$

Note: There are only two data points in the reference source.

The accuracy of this fit cannot be adequately established.

FURAN $\text{C}_4\text{H}_4\text{O}$ 45-100K

$$\text{Cp}(T) = 1099.8 + 1.3061T \quad T(\text{Cp}) = [\text{Cp} - 1099.8]/1.3061$$

Note: There are only three data points in the reference source.

The accuracy of the fit cannot be adequately established.

HELIUM He ALL TEMPERATURES

Cp(T) = 519.31 = Constant - - - - -
 n-HEPTANE - Ideal gas C₇H₁₆ 300-755K

$$\text{Cp}(T) = 94.626 + 5.860997T^4 - 1.9823132E-03T^2 - 6.886993E-08T^3 - 1.9379526E-10T$$

$$\text{Cp}(300) = 1671.09 \quad \text{Cp}(500) = 2508.83 \quad \text{Cp}(755) = 3297.1 \\ \text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

755-1365K

$$\text{Cp}(T) = -740.308 + 10.893537T^4 - 1.265124E-02T^2 + 9.843763E-06T^3 - 4.3228296E-09T^5 + 7.863665E-13T^5$$

$$\text{Cp}(755) = 3297.54 \quad \text{Cp}(1000) = 3809.29 \quad \text{Cp}(1365) = 4312.15 \\ \text{std error est} = 0.3 \quad \text{max error est} = 1.0$$

300-755K

$$\text{T(Cp)} = -194.613 + 0.4265268\text{Cp}^2 - 1.1575878E-04\text{Cp}^3 + 2.2332567E-08\text{Cp}^3 \\ \text{T(1671.09)} = 299 \quad \text{T(2508.83)} = 500 \quad \text{T(3297.1)} = 754 \\ \text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

755-1365K

$$\text{T(Cp)} = -4882.496 + 4.4329699\text{Cp}^2 - 1.260663E-03\text{Cp}^3 + 1.318505E-07\text{Cp}^3 \\ \text{T(3297.54)} = 755 \quad \text{T(3809.29)} = 999 \quad \text{T(4312.15)} = 1364$$

std error est = 0.9 - - - - - max error est = 2.5

HEXAFLUOROETHANE (CF₃)₂ 175-1175K

$$\text{Cp}(T) = 659.43 - 2.9660847T + 2.168867E-02T^2 - 4.922597E-05T^3 + 5.4905868E-08T^4 - 3.068691E-11T^5 + 6.876342E-15T^6$$

$$\text{Cp}(175) = 587.42 \quad \text{Cp}(675) = 1148.43 \quad \text{Cp}(1175) = 1286.31 \\ \text{std error est} = 4.9 \quad \text{max error est} = 11.0$$

n-HEXANE - Ideal gas C₆H₁₄ 275-755K

$$\text{Cp}(T) = 244.084 + 5.0862655T - 5.31415E-04T^2 - 1.0882839E-06T^3 \\ \text{Cp}(275) = 1579.99 \quad \text{Cp}(500) = 2518.33 \quad \text{Cp}(755) = 3312.93 \\ \text{std error est} = 0.2 \quad \text{max error est} = 1.0$$

755-1365K

$$\text{Cp}(T) = 4009.13 - 11.718687T + 0.0298761T^2 - 2.9593554E-05T^3 + 1.375164E-08T^4 - 2.4932142E-12T^5$$

$$\text{Cp}(755) = 3312.16 \quad \text{Cp}(1000) = 3831.41 \quad \text{Cp}(1365) = 4339.26 \\ \text{std error est} = 0.7 \quad \text{max error est} = 2.0$$

275-755K

$$\text{T(Cp)} = -209.84 + 0.4334954\text{Cp}^2 - 1.1488097E-04\text{Cp}^3 + 2.167164E-08\text{Cp}^3 \\ \text{T(1579.99)} = 274 \quad \text{T(2518.33)} = 499 \quad \text{T(3312.93)} = 753 \\ \text{std error est} = 0.6 \quad \text{max error est} = 2.5$$

755-1365K

$$\text{T(Cp)} = -5668.09 + 5.032992\text{Cp}^2 - 1.41023E-03\text{Cp}^3 + 1.437634E-07\text{Cp}^3 \\ \text{T(3312.16)} = 755 \quad \text{T(3831.41)} = 999 \quad \text{T(4339.26)} = 1364$$

n-HEXANE (continued)

std error est = 0.6 max error est = 2.5
CYCLOHEXANE C₆H₁₂ 300-1500K

$$Cp(T) = -143.687 + 2.2338877T + 1.5757957E-02T^2 - 3.322767E-05T^3 + 2.992193E-08T^4 - 1.3118055E-11T^5 + 2.278605E-15T^6$$

$$Cp(300) = 1259.7 \quad Cp(800) = 3270.77 \quad Cp(1500) = 4338.44$$

std error est = 2.0 max error est = 3.5

$$T(Cp) = 493.2108 - 0.6186162Cp + 5.38728E-04Cp^2 - 1.568782E-07Cp^3 + 1.7939201E-11Cp^4$$

$$T(1259.7) = 300 \quad T(3270.77) = 797 \quad T(4338.44) = 1494$$

std error est = 4.5 max error est = 10.0

HYDRAZINE N₂H₄ 275-1475K

$$Cp(T) = 164.415 + 6.9555374T - 7.864965E-03T^2 + 4.8061401E-06T^3 - 1.14436786E-09T^4$$

$$Cp(275) = 1575.81 \quad Cp(675) = 2516.48 \quad Cp(1475) = 3319.06$$

std error est = 4.3 max error est = 6.5

$$T(Cp) = -382.0766 + 0.7822092Cp - 3.7974324E-04Cp^2 + 9.376375E-08Cp^3$$
$$T(1575.81) = 274 \quad T(2516.48) = 676 \quad T(3319.06) = 1459$$

std error est = 7.5 max error est = 16.0

HYDROBROMIC ACID HBr 350-1500K

$$Cp(T) = 395.3995 - 0.2258915T + 4.5013067E-04T^2 - 2.807402E-07T^3 + 6.0719708E-11T^4$$

$$Cp(350) = 360.35 \quad Cp(850) = 387.9 \quad Cp(1500) = 429.25$$

std error est = 0.4 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 350-1500K, Cp(T) = 333.6168303 ± 6.18710596E-02T ± 2.6754517E-06T²

HYDROCYANIC ACID HCN 100-1500K

$$Cp(T) = 1044.92 - 0.430188124T + 9.2162939E-03T^2 - 2.1505599E-05T^3 + 2.29172856E-08T^4 - 1.1686957E-11T^5 + 2.3027052E-15T^6$$

$$Cp(100) = 1074.74 \quad Cp(800) = 1749.31 \quad Cp(1500) = 2055.08$$

std error est = 7.2 max error est = 16.5

$$T(Cp) = -52339.698 + 171.0170866Cp - 0.2213524775Cp^2 + 1.4203695E-04Cp^3 - 4.51189157E-08Cp^4 + 5.7079687E-12Cp^5$$

$$T(1074.74) = 95 \quad T(1749.31) = 796 \quad T(2055.08) = 1507$$

std error est = 1.5 max error est = 7.5

HYDROFLUORIC ACID HF 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 1460.773641 - 0.081301137T + 4.32324705E-04T^2 \\ & - 1.12701828E-06T^3 + 1.51594969E-09T^4 - 8.75540737E-13T^5 \\ & + 1.82375488E-16T^6 \\ \text{Cp}(100) = & 1455.98 \quad \text{Cp}(800) = 1477.23 \quad \text{Cp}(1500) = 1611.09 \\ \text{std error est} = & 0.4 \quad \text{max error est} = 1.0 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 100-1500K, $\text{Cp}(T) = 1464.2305292 - 0.0715176125T + 1.1488975E-04T^2$.

HYDROFLUORIC ACID, DF 300-1500K

MONODEUTERATED

$$\begin{aligned} \text{Cp}(T) = & 1317.953085 + 0.736930447T - 2.979053E-03T^2 + 5.585763E-06T^3 \\ & - 4.8632489E-09T^4 + 2.04262374E-12T^5 - 3.37598227E-16T^6 \\ \text{Cp}(300) = & 1387.06 \quad \text{Cp}(800) = 1449.66 \quad \text{Cp}(1500) = 1617.95 \\ \text{std error est} = & 0.4 \quad \text{max error est} = 1.5 \end{aligned}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 300-1500K, $\text{Cp}(T) = 1444.09476 - 0.35547209T + 6.1254815E-04T^2 - 1.9925363E-07T^3$.

HYDROGEN - Ideal gas H₂ 100-425K

$$\begin{aligned} \text{Cp}(T) = & 5006.6253 + 101.569422T - 0.602891517T^2 + 2.7375894E-03T^3 \\ & - 8.4758275E-06T^4 + 1.43800374E-08T^5 - 9.8072403E-12T^6 \\ \text{Cp}(100) = & 11158.65 \quad \text{Cp}(325) = 14334.47 \quad \text{Cp}(425) = 14498.83 \\ \text{std error est} = & 3.2 \quad \text{max error est} = 6.5 \\ \text{Cp}(T) = & 14920.082 - 1.996917584T + 2.540615E-03T^2 - 4.7588954E-07T^3 \\ \text{Cp}(490) = & 14495.61 \quad \text{Cp}(850) = 14766.04 \quad \text{Cp}(1365) = 15717.7 \\ \text{std error est} = & 1.3 \quad \text{max error est} = 4 \end{aligned}$$

Note: For temperatures between 425-490, Cp = 14494.7 - constant.

HYDROGEN - Real gas 100-365K

$$\begin{aligned} \text{Cp}(T) = & 6436.5105 + 63.161307T - 0.1685728T^2 + 1.5229265E-04T^3 \\ \text{Cp}(100) = & 11219.21 \quad \text{Cp}(225) = 13848.52 \quad \text{Cp}(365) = 14437.83 \\ \text{std error est} = & 1.2 \quad \text{max error est} = 2 \\ \text{Cp}(T) = & 29616.406 - 51.4939245T + 0.304123881T^2 - 4.2495904E-03T^3 \\ & + 1.9472701E-05T^4 - 3.55632306E-08T^5 + 2.30568584E-11T^6 \\ \text{Cp}(365) = & 14440.87 \quad \text{Cp}(425) = 14506.73 \quad \text{Cp}(475) = 14512.49 \end{aligned}$$

HYDROGEN - Real gas (continued)

std error est = 2.0

max error est = 4.5

475-1255K

$$Cp(T) = 15009.352 - 2.2923455T + 2.869303E-03T^2 - 5.937169E-07T^3$$

$$Cp(475) = 14504.24 \quad Cp(875) = 14802.62 \quad Cp(1255) = 15478.11$$

std error est = 1.3

max error est = 5.5

HYDROGEN (Monatomic) H 100-1500K

- Cp(T) = 20622 = constant

HYDROGEN, MONODEUTERATED HD 0-1500K

$$Cp(T) = 9648.403 + 0.180166208T - 4.410482E-04T^2 + 3.02156-1E-05T^3$$
$$- 2.37468746E-09T^4 + 5.54340759E-13T^5$$

$$Cp(1) = 9648.58 \quad Cp(800) = 10266.28 \quad Cp(1500) = 11311.73$$

- std error est = 0.6 max error est = 1.5

HYDROGEN CHLORIDE HCl 365-1365K

Ideal gas

$$Cp(T) = 770.99488 + 0.26534577T - 9.9858498E-04T^2 + 1.7010329E-06T^3$$
$$- 1.1455977E-09T^4 + 2.736703E-13T^5$$

$$Cp(365) = 798.97 \quad Cp(850) = 843.13 \quad Cp(1365) = 918.63$$

std error est = 0.3 max error est = 1.0

Note: From 255-365K, Cp = 798.84 - constant.

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 365-1365K, Cp(T) =

$$841.8819 - 0.2461627T + 4.0609005E-04T^2 - 1.3558119E-07T^3$$

HYDROGEN IODIDE - Ideal gas HI 275-1365K

$$Cp(T) = 248.5266 - 0.15405244T + 3.53994265E-04T^2 - 2.5054778E-07T^3$$
$$+ 6.12525942E-11T^4$$

$$Cp(275) = 228.07 \quad Cp(875) = 252.82 \quad Cp(1365) = 273.24$$

std error est = 0.2 max error est = 1.0

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 275-1365K, Cp(T) =

$$214.2405 + 3.60151566E-02T + 6.81264406E-06T^2$$

HYDROGEN PEROXIDE H₂O₂ 300-1500K

$$Cp(T) = 827.2894 + 1.66579757T - 6.5656617E-04T^2 + 4.920427E-08T^3$$

$$Cp(300) = 1269.27 \quad Cp(800) = 1764.92 \quad Cp(1500) = 2014.78$$

std error est = 0.6 max error est = 1.5

Note: For T(Cp) calculations, use the above equation and iteratives.

HYDROGEN SULFIDE - Ideal gas H₂S 200-1365K

$$Cp(T) = 1001.424 - 0.442935517T + 2.03071482E-03T^2 - 1.946487E-06T^3 \\ + 8.5559054E-10T^4 - 1.51906275E-13T^5$$

$$Cp(200) = 979.81 \quad Cp(800) = 1250.81 \quad Cp(1365) = 1480.42 \\ \underline{\text{std error est} = 0.4} \quad \underline{\text{max error est} = 1.5}$$

HYDROGEN SULFIDE, D₂S 100-1500K
D¹DEUTERATED

$$Cp(T) = 951.92162 - 0.636298T + 3.834902E-03T^2 - 5.1606288E-06T^3 \\ + 3.4347917E-09T^4 - 1.18396309E-12T^5 + 1.70442092E-16T^6$$

$$Cp(100) = 921.81 \quad Cp(800) = 1318.59 \quad Cp(1500) = 1548.24 \\ \underline{\text{std error est} = 0.7} \quad \underline{\text{max error est} = 1.5}$$

$$T(Cp) = -164765.798 + 671.44529Cp - 1.09343063Cp^2 + 8.8987356E-04Cp^3 \\ - 3.61561554E-07Cp^4 + 5.87557715E-11Cp^5$$

$$T(921.81) = 129 \quad T(1318.59) = 803 \quad T(1548.24) = 1505 \\ \underline{\text{std error est} = 8.5} \quad \underline{\text{max error est} = 29.0}$$

HYDROGEN SULFIDE, T₂S 50-250K
DITRITIATED

$$Cp(T) = 867.963 + 0.2747135T - 5.06698273E-03T^2 + 3.5644166E-05T^3 \\ - 6.07263928E-08T^4$$

$$Cp(50) = 873.08 \quad Cp(180) = 897.27 \quad Cp(250) = 939.54 \\ \underline{\text{std error est} = 0.5} \quad \underline{\text{max error est} = 1.5}$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 50-250K, Cp(T) = 884.648608 - 0.326396624T + 2.20660346E-03T²

HYDROGEN SULFIDE, HDS 50-1500K
MONODEUTERATED

$$Cp(T) = 962.62194 - 0.35271253T + 1.90644836E-03T^2 - 1.27551132E-06T^3 \\ - 3.3335115E-10T^4 + 6.2782923E-13T^5 - 1.75469178E-16T^6$$

$$Cp(50) = 949.59 \quad Cp(800) = 1270.71 \quad Cp(1500) = 1499.5 \\ \underline{\text{std error est} = 1.3} \quad \underline{\text{max error est} = 2.5}$$

HYDROGEN SULFIDE, MONO-DTS 100-250K
DEUTERATED/MONOTRITIATED

$$Cp(T) = 930.5966 - 0.671343T + 3.7680173E-03T^2 - 3.14889788E-06T^3$$

$$Cp(100) = 897.99 \quad Cp(175) = 911.63 \quad Cp(250) = 949.06 \\ \underline{\text{std error est} = 0.3} \quad \underline{\text{max error est} = 1.5}$$

$$T(Cp) = -1873390.367 + 6052.319684Cp - 6.51827856Cp^2 + 2.3405097E-03Cp^3 \\ T(897.99) = 109 \quad T(911.63) = 180 \quad T(949.09) = 257$$

$$\underline{\text{std error est} = 2.4} \quad \underline{\text{max error est} = 8.5}$$

HYDROGEN SULFIDE, MONO- HTS 50-1500K

TRITIATED

$$Cp(T) = 947.2175 - 0.6001111T + 3.4256972E-03T^2 - 4.2387292E-06T^3 \\ + 2.28571453E-09T^4 - 4.6662046E-13T^5$$

$$Cp(50) = 925.26 \quad Cp(800) = 1272.67 \quad Cp(1500) = 1477.19 \\ \text{std error est} = 2.2 \quad \text{max error est} = 6.5$$

HYDROXYL OH 0-1500K

$$Cp(T) = 1761.23799 - 0.2890543T + 7.1609328E-04T^2 - 3.6725166E-07T^3 \\ + 5.9334163E-11T^4$$

$$Cp(1) = 1760.95 \quad Cp(800) = 1824.56 \quad Cp(1500) = 1999.77 \\ \text{std error est} = 3.0 \quad \text{max error est} = 5.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 0-1500K, $Cp(T) = 1758.418762 - 0.236699T + 5.4753303E-04T^2 - 1.89130827E-07T^3$

IODINE I₂ 250-1500K

$$Cp(T) = 131.03309 + 8.1451251E-02T - 1.4276222E-04T^2 + 1.088693E-07T^3 \\ - 2.9318658E-11T^4$$

$$Cp(250) = 144.06 \quad Cp(900) = 148.83 \quad Cp(1500) = 151.00 \\ \text{std error est} = 0.4 \quad \text{max error est} = 1.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, $Cp(T) = 142.223033 + 1.13334775E-02T - 3.7835264E-06T^2$

IODINE (Monatomic) 55-1550K

Cp(T) = 164.50 - constant

IODINE BROMIDE IBr 250-1500K

$$Cp(T) = 160.52687 + 8.1079813E-02T - 1.175744E-04T^2 + 7.647269E-08T^3 \\ - 1.81218914E-11T^4$$

$$Cp(250) = 174.57 \quad Cp(800) = 181.87 \quad Cp(1500) = 183.96 \\ \text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, $Cp(T) = 170.84732 + 2.05167565E-02T - 8.09243496E-06T^2$

IODINE CHLORIDE ICl 250-1500K

$$Cp(T) = 186.45308 + 0.1656137T - 2.3408245E-04T^2 + 1.4813037E-07T^3 \\ - 3.44570338E-11T^4$$

IODINE CHLORIDE (continued)

Cp(250) = 215.41 Cp(800) = 230.86 Cp(1500) = 233.69
std error est = 0.4 max error est = 1.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn; 250-1500K, $C_p(T) = 207.56253 + 4.364782E-02T - 1.811719E-05T^2$.

IODINE FLUORIDE IF 250-1500K

$C_p(T) = 175.3521 + 0.26519153T - 3.3997426E-04T^2 + 1.9855293E-07T^3$
 $- 4.316987E-11T^4$
 $C_p(250) = 223.34 \quad C_p(800) = 253.9 \quad C_p(1500) = 259.77$
 std error est = 0.4 max error est = 1.5

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, $C_p(T) = 188.3318389 + 0.1798053T - 1.5965353E-04T^2 + 4.7953466E-08T^3$.

IODINE HEPTAFLUORIDE IF₇ 250-1000K

$C_p(T) = -386.25397 + 6.988192T - 2.19E-02T^2 + 3.9399594E-05T^3$
 $- 4.11419754E-08T^4 + 2.31307177E-11T^5 - 5.40722595E-15T^6$
 $C_p(250) = 468.22 \quad C_p(600) = 647.34 \quad C_p(1000) = 683.05$
 std error est = 0.5 max error est = 1.5

IODINE PENTAFLUORIDE IF_5 250-1500K

$$\begin{aligned} Cp(T) &= -58.2197 + 3.228146T - 7.466701E-03T^2 + 9.66136789E-06T^3 \\ &\quad - 7.133844E-09T^4 + 2.80488185E-12T^5 - 4.551596E-16T^6 \\ Cp(250) &= 407.87 \quad Cp(800) = 569.99 \quad Cp(1500) = 590.97 \\ \text{std error est} &= 0.5 \quad \text{max error est} = 1.5 \end{aligned}$$

IODOMETHANE CH_3I 300–600K

$C_p(T) = 238.1717 \exp(0.0011T)$ max error est = 5.0%
 ISOPRENE $\text{CH}_3\text{C}(\text{CH}_3)\text{CHCH}_3$ 275-1500K

ISOPRENE $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_3$ 275-1500K

$$C_p(T) = -396.2635 + 8.948094T - 1.0120624E-02T^2 + 7.068983E-06T^3 - 2.65012106E-09T^4 + 3.98613124E-13T^5$$

$$C_p(275) = 1431.57 \quad C_p(900) = 3109.24 \quad C_p(1500) = 3723.02$$

std error est = 1.9 max error est = 4.5

275-1500K

$$T(Cp) = 1061.69 - 1.77172Cp + 1.3189685E-03Cp^2 - 3.9005614E-07Cp^3 + 4.618566E-11Cp^4$$

$$T(1431.57) = 278 \quad T(3109.24) = 896 \quad T(3723.02) = 1492$$

std error est = 4.4 max error est = 8.5

KETENE H₂CCO 250-1500K

$$\begin{aligned} \text{Cp}(T) &= 399.1048 + 2.617846T + 5.971587E-04T^2 - 5.279979E-06T^3 \\ &\quad + 6.195382E-09T^4 - 3.1370787E-12T^5 + 6.0082048E-16T^6 \\ \text{Cp}(250) &= 1029.67 \quad \text{Cp}(800) = 1839.39 \quad \text{Cp}(1500) = 2235.20 \\ \text{std error est} &= 1.0 \quad \text{max error est} = 2.5 \end{aligned}$$

250-1500K

$$\begin{aligned} \text{T(Cp)} &= 2213.102 - 6.36729113\text{Cp} + 7.14666E-03\text{Cp}^2 - 3.3641974E-06\text{Cp}^3 \\ &\quad + 6.1602663E-10\text{Cp}^4 \\ \text{T}(1029.67) &= 254 \quad \text{T}(1839.39) = 796 \quad \text{T}(2235.20) = 1494 \\ \text{- std error est} &= 4.0 \quad \text{- max error est} = 8.5 \end{aligned}$$

KRYPTON Kr ALL TEMPERATURES

- Cp(T) = 248.05 - constant

MESITYLENE C₆H₃(CH₃)₃ 300-1500K

$$\begin{aligned} \text{Cp}(T) &= 240.097 + 2.177066T + 7.26309147E-03T^2 - 1.36166E-05T^3 \\ &\quad + 9.1161133E-09T^4 - 2.1807381E-12T^5 \\ \text{Cp}(300) &= 1247.79 \quad \text{Cp}(800) = 2677.81 \quad \text{Cp}(1500) = 3481.97 \\ \text{std error est} &= 1.5 \quad \text{max error est} = 2.5 \end{aligned}$$

300-1500K

$$\begin{aligned} \text{T(Cp)} &= 439.7914 - 0.759142\text{Cp} + 8.223984E-04\text{Cp}^2 - 2.963892E-07\text{Cp}^3 \\ &\quad + 4.24823947E-11\text{Cp}^4 \\ \text{T}(1247.79) &= 300 \quad \text{T}(2677.81) = 797 \quad \text{T}(3481.97) = 1500 \\ \text{- std error est} &= 2.9 \quad \text{- max error est} = 4.5 \end{aligned}$$

METHANE - Ideal gas CH₄ 275-755K

$$\begin{aligned} \text{Cp}(T) &= 1916.5258 - 1.09269T + 8.696605E-03T^2 - 5.2291144E-06T^3 \\ \text{Cp}(275) &= 2164.97 \quad \text{Cp}(500) = 2890.69 \quad \text{Cp}(755) = 3799.38 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

755-1365K

$$\begin{aligned} \text{Cp}(T) &= 10435.6 - 42.025284T + 8.849006E-02T^2 - 8.4304566E-05T^3 \\ &\quad + 3.9030203E-08T^4 - 7.1345169E-12T^5 \\ \text{Cp}(755) &= 3797.77 \quad \text{Cp}(1000) = 4491.5 \quad \text{Cp}(1365) = 5224.89 \\ \text{std error est} &= 1.0 \quad \text{max error est} = 2.5 \end{aligned}$$

275-755K

$$\begin{aligned} \text{T(Cp)} &= -1405.54 + 1.36736\text{Cp} - 3.55452E-04\text{Cp}^2 + 3.823585E-08\text{Cp}^3 \\ \text{T}(2164.97) &= 277 \quad \text{T}(2890.69) = 500 \quad \text{T}(3799.38) = 756 \\ \text{std error est} &= 0.5 \quad \text{max error est} = 2.5 \end{aligned}$$

755-1365K

$$\begin{aligned} \text{T(Cp)} &= -2892.182 + 2.2452\text{Cp} - 5.10113E-04\text{Cp}^2 + 4.52369E-08\text{Cp}^3 \\ \text{T}(3797.77) &= 755 \quad \text{T}(4491.5) = 1000 \quad \text{T}(5224.89) = 1365 \\ \text{std error est} &= 0.4 \quad \text{max error est} = 2.5 \end{aligned}$$

METHANE - Real gas

METHANE - Real gas (continued) 275-510K

$$Cp(T) = -12236.8831 + 262.518875T - 1.9826045T^2 + 7.840392E-03T^3 \\ - 1.70541464E-05T^4 + 1.9431809E-08T^5 - 9.08114724E-12T^6$$

$$Cp(275) = 2175.89 \quad Cp(375) = 2457.67 \quad Cp(510) = 2912.87 \\ \text{std error est} = 2.7 \quad \text{max error est} = 6.5$$

275-510K

$$T(Cp) = -742.678 + 0.58853377Cp - 5.46177054E-05Cp^2$$

$$T(2175.89) = 279 \quad T(2457.67) = 374 \quad T(2912.87) = 508$$

$$- \text{std error est} = 2.8 \quad - \text{max error est} = 5.5$$

METHANE, DIDEUTERATED CH_2D_2 95-1275K

$$\ln[Cp(T)] = 7.6070340658 - 1.74744883E-03T + 9.23134494E-06T^2 \\ - 1.06684914E-08T^3 + 3.85790574E-12T^4$$

$$Cp(95) = 1836.3 \quad Cp(675) = 3475.02 \quad Cp(1275) = 4762.75$$

$$- \text{**Note: } Cp(T) = \exp[fctn(T)] \quad - \text{max error est} = 45.0$$

METHANE, DIDEUTERATED CD_2T_2 95-1275K

DITRITIATED

$$Cp(T) = 1858.141 - 6.9817888T + 4.033067E-02T^2 - 6.835852E-05T^3 \\ + 5.20572E-08T^4 - 1.490558E-11T^5$$

$$Cp(95) = 1504.37 \quad Cp(675) = 3215.76 \quad Cp(1275) = 4180.76$$

$$- \text{std error est} = 3.0 \quad - \text{max error est} = 6.5$$

METHANE, DITRITIATED CH_2T_2 95-1275K

$$Cp(T) = 1861.969 - 3.8411072T + 1.9495867E-02T^2 - 2.0658472E-05T^3 \\ + 7.0155845E-09T^4$$

$$Cp(95) = 1655.87 \quad Cp(675) = 3254.97 \quad Cp(1275) = 4379.07$$

$$- \text{std error est} = 7.2 \quad - \text{max error est} = 15.0$$

METHANE, MONODEUTERATED CH_3D 95-1275K

$$\ln[Cp(T)] = 7.685260605 - 1.89630346E-03T + 8.85273067E-06T^2 \\ - 9.69191539E-09T^3 + 3.378275E-12T^4$$

$$Cp(95) = 1952.7 \quad Cp(675) = 3495.99 \quad Cp(1275) = 4905.71$$

$$- \text{**Note: } Cp(T) = \exp[fctn(T)] \quad - \text{max error est} = 9.5$$

METHANE, MONODEUTERATED, CDT_3 95-1275K

TRITRITIATED

$$Cp(T) = 1792.8646 - 7.153158T + 4.2595806E-02T^2 - 7.46524585E-05T^3 \\ + 5.84466516E-08T^4 - 1.70935846E-11T^5$$

$$Cp(95) = 1438.36 \quad Cp(675) = 3150.99 \quad Cp(1275) = 4046.87$$

$$- \text{std error est} = 1.2 \quad - \text{max error est} = 2.5$$

METHANE, MONOTRITIATED CH_3T 95-1275K

$$\ln[Cp(T)] = 7.623967385 - 1.89530858E-03T + 9.19540139E-06T^2 \\ - 1.02844644E-08T^3 + 3.63747258E-12T^4$$

METHANE, MONOTRITIATED (continued)

$C_p(95) = 1841.58$ $C_p(675) = 3382.78$ $C_p(1275) = 4684.41$
~~- **Note: $C_p(T) = \exp[fctn(T)]$~~ ~~max error est = 11.5~~

METHANE, TETRADEUTERATED CD_4 95-1275K

$\ln[C_p(T)] = 7.6175941054 - 4.03359764E-03T + 2.34289511E-05T^2$
 $- 4.27574857E-08T^3 + 3.43557214E-11T^4 - 1.01858966E-14T^5$
 $C_p(95) = 1655.58$ $C_p(675) = 3376.31$ $C_p(1275) = 4488.86$
~~- **Note: $C_p(T) = \exp[fctn(T)]$~~ ~~max error est = 15.0~~

METHANE, TETRATRITIATED CT_4 95-1275K

$C_p(T) = 1736.415 - 7.3850897T + 4.525255E-02T^2 - 8.1987002E-05T^3$
 $+ 6.5925034E-08T^4 - 1.9662464E-11T^5$
 $C_p(95) = 1378.16$ $C_p(675) = 3085.25$ $C_p(1275) = 3918.72$
~~- std error est = 2.9~~ ~~max error est = 9.5~~

METHANE, TRIDEUTERATED CHD_3 95-1275K

$C_p(T) = 1967.71 - 4.14269394T + 2.0693509E-02T^2 - 2.1823919E-05T^3$
 $+ 7.39241354E-09T^4$
 $C_p(95) = 1742.80$ $C_p(675) = 3422.62$ $C_p(1275) = 4627.45$
~~- std error est = 8.8~~ ~~max error est = 15.0~~

METHANE, TRIDEUTERATED, CD_3T 95-1275K
 MONOTRITIATED

$C_p(T) = 1909.6275 - 6.445028T + 3.602721E-02T^2 - 5.7366078E-05T^3$
 $+ 4.11246853E-08T^4 - 1.11879465E-11T^5$
 $C_p(95) = 1576.57$ $C_p(675) = 3300.89$ $C_p(1275) = 4339.79$
~~- std error est = 5.3~~ ~~max error est = 11.0~~

METHANE, TRITRITIATED CHT_3 95-1275K

$C_p(T) = 1793.405 - 5.700601T + 3.260151E-02T^2 - 5.1462346E-05T^3$
 $+ 3.64062843E-08T^4 - 9.77635312E-12T^5$
 $C_p(95) = 1504.84$ $C_p(675) = 3160.29$ $C_p(1275) = 4127.4$
~~- std error est = 3.6~~ ~~max error est = 6.5~~

METHANETHIOL CH_3SH 300-1000K

$C_p(T) = 706.9902 + 0.0461346T + 6.2988574E-03T^2 - 1.0655555E-05T^3$
 $+ 7.67648136E-09T^4 - 2.11193895E-12T^5$
 $C_p(300) = 1057.08$ $C_p(700) = 1659.04$ $C_p(1000) = 1960.97$
~~std error est = 0.5~~ ~~max error est = 2.5~~

300-1000K

 $T(C_p) = -689.19 + 1.5805785C_p - 8.9447465E-04C_p^2 + 2.6908387E-07C_p^3$
 $T(1057.08) = 300$ $T(1659.04) = 700$ $T(1960.97) = 1000$
~~- std error est = 0.4~~ ~~max error est = 1.5~~

2-METHYL-2-BUTANOL $(\text{CH}_3)_2\text{COHCH}_2\text{CH}_3$ 400-575K

$$\ln[\text{Cp}(T)] = 722.5726607 - 5.769804449T + 0.012524666T^2 + 1.60592914E-05T^3 - 1.06765564E-07T^4 + 1.57879296E-10T^5 - 7.86807765E-14T^6$$

$$\text{Cp}(400) = 2000.65 \quad \text{Cp}(500) = 2301.88 \quad \text{Cp}(575) = 2736.30$$

- **Note: $\text{Cp}(T) = \exp[f_{\text{ctn}}(T)]$ - - - - - max_error_est = 10.0

3-METHYL-1-BUTANOL $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{OH}$ 450-500K

$$\text{Cp}(T) = 12449.8133 - 46.47211274T + 5.25188485E-02T^2$$
$$\text{Cp}(450) = 2172.43 \quad \text{Cp}(475) = 2225.12 \quad \text{Cp}(500) = 2343.47$$

std error est = 1.1 max error est = 4.5

450-500K

$$T(\text{Cp}) = -6275.55 + 5.7093249\text{Cp} - 1.20269088E-03\text{Cp}^2$$
$$T(2172.43) = 452 \quad T(2225.12) = 474 \quad T(2343.47) = 499$$

- std error est = 2.4 - - - - - max_error_est = 6.0

3-METHYL-1-BUTYNE $(\text{CH}_3)_2\text{CHCCH}$ 300-1500K

$$\text{Cp}(T) = 17.777 + 6.352748T - 4.78347376E-03T^2 + 1.9843222E-06T^3 - 3.49882302E-10T^4$$
$$\text{Cp}(300) = 1543.83 \quad \text{Cp}(800) = 2911.21 \quad \text{Cp}(1500) = 3709.89$$

std error est = 2.0 max error est = 4.5

300-1500K

$$T(\text{Cp}) = 1134.29 - 1.94512287\text{Cp} + 1.4522943E-03\text{Cp}^2 - 4.2842051E-07\text{Cp}^3 + 4.99658252E-11\text{Cp}^4$$
$$T(1543.83) = 300 \quad T(2911.21) = 799 \quad T(3709.89) = 1496$$

- std error est = 2.9 - - - - - max_error_est = 6.5

METHYL CHLORIDE CH_3Cl 255-755K

Ideal gas

$$\text{Cp}(T) = 332.8997 + 1.6366402T - 3.801244E-05T^2 - 4.04253913E-07T^3$$
$$\text{Cp}(275) = 771.69 \quad \text{Cp}(500) = 1091.19 \quad \text{Cp}(755) = 1372.92$$

std error est = 0.2 max error est = 2.5

755-1365K

$$\text{Cp}(T) = 526.238 + 1.16955813T + 2.7488708E-04T^2 - 5.75072686E-07T^3 + 1.67250614E-10T^4$$
$$\text{Cp}(755) = 1372.8 \quad \text{Cp}(1000) = 1562.86 \quad \text{Cp}(1365) = 1752.91$$

std error est = 0.1 max error est = 1.0

255-755K

$$T(\text{Cp}) = -458.583 + 1.4667588\text{Cp} - 9.82376432E-04\text{Cp}^2 + 4.05810172E-07\text{Cp}^3$$
$$T(771.69) = 275 \quad T(1091.19) = 499 \quad T(1372.92) = 754$$

std error est = 0.5 max error est = 1.5

755-1365K

$$\text{Cp}(T) = -6942.55 + 14.831976\text{Cp} - 1.0193339E-02\text{Cp}^2 + 2.5303315E-06\text{Cp}^3$$
$$T(1372.8) = 755 \quad T(1562.86) = 999 \quad T(1752.91) = 1364$$

std error est = 0.6 max error est = 1.5

METHYL CYANIDE CH₃CN 290-1200K

$$Cp(T) = 1303.384 - 4.942871T + 2.849223E-02T^2 - 5.4871983E-05T^3 \\ + 5.3623977E-08T^4 - 2.63165765E-11T^5 + 5.11566313E-15T^6$$

$$Cp(290) = 1256.21 \quad Cp(650) = 1963.81 \quad Cp(1200) = 2567.87 \\ \text{std error est} = 1.7 \quad \text{max error est} = 4.5$$

290-1200K

$$T(Cp) = -813.42 + 1.58371Cp - 8.002791E-04Cp^2 + 1.8985947E-07Cp^3 \\ T(1256.21) = 290 \quad T(1963.81) = 648 \quad T(2567.87) = 1192$$

$$\text{std error est} = 4.4 \quad \text{max error est} = 9.5$$

METHYL ETHER (CH₃)₂O 275-1275K

$$Cp(T) = 626.107 + 2.175166T + 2.77749E-03T^2 - 3.7041748E-06T^3 \\ + 1.1994434E-09T^4$$

$$Cp(275) = 1364.15 \quad Cp(675) = 2469.63 \quad Cp(1275) = 3406.78 \\ \text{std error est} = 7.2 \quad \text{max error est} = 15.5$$

275-1275K

$$T(Cp) = -687.49 + 1.161406Cp - 4.4639784E-04Cp^2 + 8.05362496E-08Cp^3 \\ T(1364.15) = 271 \quad T(2469.63) = 671 \quad T(3406.78) = 1273$$

$$\text{std error est} = 6.3 \quad \text{max error est} = 10.5$$

METHYLHYDRAZINE CH₃NHNH₂ 300-1500K

$$Cp(T) = -230.3353 + 8.3735806T - 1.038813E-02T^2 + 8.570289E-06T^3 \\ - 3.9110406E-09T^4 + 7.27987797E-13T^5$$

$$Cp(300) = 1548.29 \quad Cp(800) = 2844.7 \quad Cp(1500) = 3609.98 \\ \text{std error est} = 5.1 \quad \text{max error est} = 10.5$$

300-1500K

$$T(Cp) = 1646.485 - 2.833585Cp + 2.0125928E-03Cp^2 - 5.8370013E-07Cp^3 \\ + 6.66115245E-11Cp^4$$

$$T(1548.29) = 300 \quad T(2844.7) = 798 \quad T(3609.98) = 1498 \\ \text{std error est} = 4.7 \quad \text{max error est} = 7.5$$

METHYLLIDYNE CH 300-1000K

$$Cp(T) = 2156.83 + 0.2622T \quad T(Cp) = [Cp - 2156.83]/0.2622$$

Note: There are only two data points in the reference source.

The accuracy of the fit cannot be adequately established.

METHYL ISOCYANIDE CH₃NC 275-755K

$$Cp(T) = 357.656 + 6.2401786T - 2.013433E-02T^2 + 4.623548E-05T^3 \\ - 5.0729918E-08T^4 + 2.0834756E-11T^5$$

$$Cp(275) = 1255.24 \quad Cp(500) = 1704.06 \quad Cp(755) = 2117.84 \\ \text{std error est} = 1.7 \quad \text{max error est} = 20.0$$

METHYL ISOCYANIDE (continued) 275-755K

$T(Cp) = -929.29 + 1.6998Cp - 8.2667574E-04Cp^2 + 1.88543E-07Cp^3$
 $T(1255.24) = 275 \quad Cp(1704.06) = 500 \quad Cp(2117.84) = 754$
- std error est = 0.9 max error est = 3.5

2-METHYLPENTANE $(CH_3)_2CH(CH_2)_2CH_3$ 300-1000K

$Cp(T) = 684.245 - 5.70106E-03T + 1.9830116E-02T^2 - 3.690549E-05T^3$
 $+ 2.8436028E-08T^4 - 8.1932667E-12T^5$

$Cp(300) = 1681.22 \quad Cp(600) = 2896.28 \quad Cp(1000) = 3845.93$
std error est = 2.0 max error est = 4.5

300-1000K

$T(Cp) = -220.405 + 0.475071Cp - 1.430724E-04Cp^2 + 2.652954E-08Cp^3$
 $T(1681.22) = 300 \quad T(2896.28) = 600 \quad T(3845.93) = 1000$
- std error est = 0.6 max error est = 2.5

3-METHYLPENTANE $[CH_3CH_2]_2CH(CH_3)$ 300-1000K

$Cp(T) = 1424.458 - 8.421426T + 6.009702E-02T^2 - 1.35448706E-04T^3$
 $+ 1.5779472E-07T^4 - 9.48522387E-11T^5 + 2.3256203E-14T^6$

$Cp(300) = 1714.25 \quad Cp(600) = 2909.14 \quad Cp(1000) = 3850.03$
std error est = 1.4 max error est = 3.5

300-1000K

$T(Cp) = -226.975 + 0.4721466Cp - 1.4127356E-04Cp^2 + 2.633499E-08Cp^3$
 $T(1714.25) = 300 \quad T(2909.14) = 599 \quad T(3850.03) = 1000$
- std error est = 0.7 max error est = 2.5

4-METHYL-2-PENTANONE $CH_3COCH_2CH(CH_3)_2$ 275-1275K

$Cp(T) = 266.655 + 4.794024T - 2.2291946E-03T^2 + 3.4395827E-07T^3$
 $Cp(275) = 1423.58 \quad Cp(675) = 2592.73 \quad Cp(1275) = 3468.11$
std error est = 7.0 max error est = 15.5

275-1275K

$T(Cp) = 892.053 - 1.68075Cp + 1.3909914E-03Cp^2 - 4.3712435E-07Cp^3$
 $+ 5.3282889E-11Cp^4$

$T(1423.58) = 275 \quad T(2592.73) = 674 \quad T(3468.11) = 1268$
- std error est = 8.1 max error est = 17.5

2-METHYL-1-PROPANOL $(CH_3)_2CHCH_2OH$ 390-600K

$Cp(T) = 66430.768 - 523.644673T + 1.572952115T^2 - 2.07471664E-03T^3$
 $+ 1.01994038E-06T^4$

$Cp(390) = 1980.96 \quad Cp(500) = 2253.15 \quad Cp(600) = 2552.20$
std error est = 8.1 max error est = 15.5

390-600K

$T(Cp) = -585.026 + 0.6296626Cp - 6.49129487E-05Cp^2$
 $T(1980.96) = 407 \quad T(2253.15) = 504 \quad T(2552.20) = 599$
- std error est = 7.9 max error est = 17.5

2-METHYL-2-PROPANOL $(\text{CH}_3)_3\text{COH}$ 360-590K

$$\begin{aligned}\text{Cp}(\text{T}) = & 1159558.4 - 14251.01382\text{T} + 72.825463058\text{T}^2 - 0.1978064\text{T}^3 \\ & + 3.0125819\text{E}-04\text{T}^4 - 2.4393359\text{E}-07\text{T}^5 + 8.2046497\text{E}-11\text{T}^6 \\ \text{Cp}(360) = & 2123.03 \quad \text{Cp}(450) = 2152.98 \quad \text{Cp}(590) = 2625.67 \\ \underline{\text{std error est}} = & 3.9 \quad \underline{\text{max error est}} = 10.5\end{aligned}$$

2-METHYLPROPENE $(\text{CH}_3)_2\text{CCH}_2$ 275-1500K

$$\begin{aligned}\text{Cp}(\text{T}) = & 360.3445 + 3.60460787\text{T} + 4.45078\text{E}-03\text{T}^2 - 1.2087027\text{E}-05\text{T}^3 \\ & + 1.1350898\text{E}-08\text{T}^4 - 5.08523225\text{E}-12\text{T}^5 + 8.992065\text{E}-16\text{T}^6 \\ \text{Cp}(275) = & 1494.14 \quad \text{Cp}(800) = 3122.69 \quad \text{Cp}(1500) = 4078.26 \\ \underline{\text{std error est}} = & 1.1 \quad \underline{\text{max error est}} = 8.0 \\ \underline{\text{275-1500K}} \\ \text{T}(\text{Cp}) = & 675.5 - 1.08191523\text{Cp} + 8.400338\text{E}-04\text{Cp}^2 - 2.3638415\text{E}-07\text{Cp}^3 \\ & + 2.637218\text{E}-11\text{Cp}^4 \\ \text{T}(1494.14) = & 277 \quad \text{T}(3122.69) = 798 \quad \text{T}(4078.26) = 1496 \\ \underline{\text{std error est}} = & 2.8 \quad \underline{\text{max error est}} = 5.5\end{aligned}$$

METHYL SULFIDE $(\text{CH}_3)_2\text{S}$ 300-1000K

$$\begin{aligned}\text{Cp}(\text{T}) = & -275.0796 + 10.650717\text{T} - 3.669097\text{E}-02\text{T}^2 + 8.1787615\text{E}-05\text{T}^3 \\ & - 9.94226515\text{E}-08\text{T}^4 + 6.1455998\text{E}-11\text{T}^5 - 1.51906388\text{E}-14\text{T}^6 \\ \text{Cp}(300) = & 1159.15 \quad \text{Cp}(600) = 1757.63 \quad \text{Cp}(1000) = 2314.99 \\ \underline{\text{std error est}} = & 0.7 \quad \underline{\text{max error est}} = 2.5 \\ \underline{\text{300-1000K}} \\ \text{T}(\text{Cp}) = & -553.78 + 1.1759729\text{Cp} - 5.4085555\text{E}-04\text{Cp}^2 + 1.3944132\text{E}-07\text{Cp}^3 \\ \text{T}(1159.15) = & 300 \quad \text{T}(1757.63) = 599 \quad \text{T}(2314.99) = 1000 \\ \underline{\text{std error est}} = & 1.0 \quad \underline{\text{max error est}} = 2.5\end{aligned}$$

NEON Ne Ideal gas ALL TEMPERATURES

$$\underline{\text{Cp}(\text{T}) = 1029.91 - \text{constant}}$$

NITRIC OXIDE - Ideal gas NO 110-1365K

$$\begin{aligned}\text{Cp}(\text{T}) = & 1188.304 - 1.4425597\text{T} + 3.465558\text{E}-03\text{T}^2 - 2.861451\text{E}-06\text{T}^3 \\ & + 4.0387214\text{E}-10\text{T}^4 + 6.1972525\text{E}-13\text{T}^5 - 2.4090578\text{E}-16\text{T}^6 \\ \text{Cp}(110) = & 1067.82 \quad \text{Cp}(800) = 1092.5 \quad \text{Cp}(1365) = 1179.32 \\ \underline{\text{std error est}} = & 0.3 \quad \underline{\text{max error est}} = 2.5\end{aligned}$$

NITRIC OXIDE - Real gas 165-645K

$$\begin{aligned}\text{Cp}(\text{T}) = & 1378.8188 - 3.82241\text{T} + 1.7887256\text{E}-02\text{T}^2 - 5.6028657\text{E}-05\text{T}^3 \\ & + 1.16489\text{E}-07\text{T}^4 - 1.32980437\text{E}-10\text{T}^5 + 6.13527678\text{E}-14\text{T}^6 \\ \text{Cp}(165) = & 1054.73 \quad \text{Cp}(400) = 997.68 \quad \text{Cp}(645) = 1054.39 \\ \underline{\text{std error est}} = & 0.3 \quad \underline{\text{max error est}} = 1.5\end{aligned}$$

NITRIC OXIDE - Real gas (continued) 645-1365K

$$\begin{aligned} \text{Cp}(T) &= 806.451 + 0.506398T - 2.0853977E-04T^2 + 2.8257004E-08T^3 \\ \text{Cp}(645) &= 1053.90 \quad \text{Cp}(1000) = 1132.57 \quad \text{Cp}(1365) = 1180.99 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.5 \end{aligned}$$

645-1365K

$$\begin{aligned} \text{T(Cp)} &= -152350.55 + 425.34707\text{Cp} - 0.39764893\text{Cp}^2 + 1.2506075E-04\text{Cp}^3 \\ \text{T}(1053.90) &= 645 \quad \text{T}(1132.57) = 998 \quad \text{T}(1180.99) = 1361 \\ \text{std error est} &= 2.0 \quad \text{max error est} = 4.5 \end{aligned}$$

NITROGEN - Ideal gas N₂ 255-590K

$$\begin{aligned} \text{Cp}(T) &= 1088.047 - 0.355968T + 7.2907605E-04T^2 - 2.8861556E-07T^3 \\ \text{Cp}(255) &= 1039.9 \quad \text{Cp}(450) = 1049.2 \quad \text{Cp}(590) = 1072.54 \\ \text{std error est} &= 0.1 \quad \text{max error est} = 1.0 \end{aligned}$$

590-1365K

$$\begin{aligned} \text{Cp}(T) &= 1405.5077 - 2.1894566T + 4.7852898E-03T^2 - 4.540166E-06T^3 \\ &\quad + 2.08491259E-09T^4 - 3.7903033E-13T^5 \\ \text{Cp}(590) &= 1072.57 \quad \text{Cp}(1000) = 1167.06 \quad \text{Cp}(1365) = 1227.83 \\ \text{std error est} &= 0.1 \quad \text{max error est} = 1.5 \end{aligned}$$

Note: For T(Cp) calculations from 255-590K, use the iterative procedures discussed in Section 5 and the following eqn: 255-590K,
 $\text{Cp}(T) = 1068.513739 - 0.20687009T + 3.63655082E-04T^2$.

590-1365K

$$\begin{aligned} \text{Cp}(T) &= -126050.925 + 333.06633\text{Cp} - 0.295083212\text{Cp}^2 + 8.823403E-05\text{Cp}^3 \\ \text{T}(1072.57) &= 592 \quad \text{T}(1167.06) = 1000 \quad \text{T}(1227.83) = 1365 \\ \text{std error est} &= 0.8 \quad \text{max error est} = 4.5 \end{aligned}$$

NITROGEN - Real gas 255-1365K

$$\begin{aligned} \text{Cp}(T) &= 1058.5365 - 4.391145E-03T - 7.6852515E-04T^2 + 2.751091E-06T^3 \\ &\quad - 3.1245817E-09T^4 + 1.5407594E-12T^5 - 2.8488096E-16T^6 \\ \text{Cp}(255) &= 1041.43 \quad \text{Cp}(800) = 1122.09 \quad \text{Cp}(1365) = 1228.69 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.0 \end{aligned}$$

NITROGEN (Monatomic) N 50-1500K

Cp(T) = 1485.0 - constant

NITROUS OXIDE - Ideal gas N₂O 200-1365K

$$\begin{aligned} \text{Cp}(T) &= 419.153 + 2.2147124T - 2.922847E-03T^2 + 2.51402093E-06T^3 \\ &\quad - 1.21894601E-09T^4 + 2.4536593E-13T^5 \\ \text{Cp}(200) &= 763.42 \quad \text{Cp}(800) = 1188.6 \quad \text{Cp}(1365) = 1321.25 \\ \text{std error est} &= 0.2 \quad \text{max error est} = 1.5 \end{aligned}$$

NITROUS OXIDE (continued) 200-1365K

$$T(Cp) = 14575.3 - 61.673304Cp + 9.760584E-02Cp^2 - 6.8073563E-05Cp^3 + 1.8008804E-08Cp^4$$

$$T(763.42) = 207 \quad Cp(1188.6) = 798 \quad Cp(1321.25) = 1349 \\ \text{std error est} = 4.5 \quad \text{max error est} = 15.5$$

n-NONANE - Ideal gas C₉H₂₀ 275-755K

$$Cp(T) = 234.445 + 5.1354876T - 6.79961E-04T^2 - 1.0363492E-06T^3$$

$$Cp(275) = 1573.73 \quad Cp(500) = 2502.65 \quad Cp(755) = 3278.13 \\ \text{std error est} = 0.2 \quad \text{max error est} = 10$$

755-1365K

$$Cp(T) = 4090.2728 - 12.293253T + 3.122246E-02T^2 - 3.12285246E-05T^3 + 1.46875287E-08T^4 - 2.6962143E-12T^5$$

$$Cp(755) = 3277.62 \quad Cp(1000) = 3782.27 \quad Cp(1365) = 4273.54 \\ \text{std error est} = 0.5 \quad \text{max error est} = 1.5$$

275-755K

$$T(Cp) = -224.99 + 0.4584096Cp - 1.27932559E-04Cp^2 + 2.413833E-08Cp^3$$

$$T(1573.73) = 274 \quad T(2502.65) = 499 \quad T(3278.13) = 753 \\ \text{std error est} = 0.7 \quad \text{max error est} = 4.5$$

755-1365K

$$T(Cp) = -5895.99 + 5.3023838Cp - 1.510136E-03Cp^2 + 1.5605569E-07Cp^3$$

$$T(3277.62) = 755 \quad T(3782.27) = 999 \quad T(4273.54) = 1364 \\ \text{std error est} = 0.6 \quad \text{max error est} = 2.5$$

n-OCTANE - Ideal gas C₈H₁₈ 275-755K

$$Cp(T) = 214.4198 + 5.356905T - 1.17497E-03T^2 - 6.991155E-07T^3$$

$$Cp(275) = 1584.17 \quad Cp(500) = 2511.74 \quad Cp(755) = 3288.24 \\ \text{std error est} = 0.2 \quad \text{max error est} = 2.5$$

755-1365K

$$Cp(T) = 2435.9686 - 4.4681947T + 1.6684329E-02T^2 - 1.7885605E-05T^3 + 8.6428202E-09T^4 - 1.614265E-12T^5$$

$$Cp(755) = 3287.84 \quad Cp(1000) = 3795.05 \quad Cp(1365) = 4289.93 \\ \text{std error est} = 0.3 \quad \text{max error est} = 2.5$$

275-755K

$$T(Cp) = -200.8856 + 0.42218566Cp - 1.119355E-04Cp^2 + 2.1840378E-08Cp^3$$

$$T(1584.17) = 274 \quad T(2511.74) = 499 \quad T(3288.24) = 754 \\ \text{std error est} = 0.6 \quad \text{max error est} = 3.5$$

755-1365K

$$T(Cp) = -5575.87 + 5.022854Cp - 1.42858E-03Cp^2 + 1.47978204E-07Cp^3$$

$$T(3287.84) = 755 \quad T(3795.05) = 999 \quad T(4289.93) = 1364 \\ \text{std error est} = 0.7 \quad \text{max error est} = 2.5$$

OXYGEN - Ideal gas O₂ 255-590K

$$Cp(T) = 929.247 - 0.3220603T + 1.166523E-03T^2 - 7.1157865E-07T^3$$

$$Cp(255) = 911.18 \quad Cp(375) = 934.99 \quad Cp(590) = 999.15$$

OXYGEN - Ideal gas (continued)

std error est = 0.1 max error est = 1.5

590-1365K

$$Cp(T) = 597.7293 + 1.183704T - 1.156226E-03T^2 + 5.82171E-07T^3 - 1.1772692E-10T^4$$

$$Cp(590) = 998.93 \quad Cp(1000) = 1089.65 \quad Cp(1365) = 1131.11 \\ \text{std error est} = 0.2 \qquad \qquad \qquad \text{max error est} = 1.5$$

255-590K

$$T(Cp) = -236734.7 + 726.57886Cp - 0.744909Cp^2 + 2.5566076E-04Cp^3$$

$$T(911.18) = 258 \quad T(934.99) = 376 \quad T(999.15) = 593$$

$$\text{std error est} = 0.9 \qquad \qquad \qquad \text{max error est} = 3.0$$

590-1365K

$$T(Cp) = -140010.9 + 416.5007Cp - 0.4145086Cp^2 + 1.386105E-04Cp^3$$

$$T(998.93) = 588 \quad T(1089.65) = 999 \quad T(1131.11) = 1361$$

$$\text{std error est} = 1.3 \qquad \qquad \qquad \text{max error est} = 5.5$$

OXYGEN - Real gas

255-590K

$$Cp(T) = 953.3639 - 0.4638376T + 1.4358763E-03T^2 - 8.748782E-07T^3$$

$$Cp(255) = 913.95 \quad Cp(450) = 955.68 \quad Cp(590) = 999.85$$

$$\text{std error est} = 0.2 \qquad \qquad \qquad \text{max error est} = 1.5$$

590-1365K

$$Cp(T) = 219.422 + 3.319747T - 5.8573E-03T^2 + 5.63507E-06T^3 - 2.77339408E-09T^4 + 5.4687139E-13T^5$$

$$Cp(590) = 999.51 \quad Cp(1000) = 1090.42 \quad Cp(1365) = 1132.44$$

$$\text{std error est} = 0.3 \qquad \qquad \qquad \text{max error est} = 2.5$$

255-590K

$$T(Cp) = -295718.67 + 907.2036Cp - 0.92916735Cp^2 + 3.182752E-04Cp^3$$

$$T(913.95) = 262 \quad T(955.68) = 452 \quad T(999.85) = 592$$

$$\text{std error est} = 2.7 \qquad \qquad \qquad \text{max error est} = 6.5$$

590-1365K

$$T(Cp) = -132405.2 + 394.1196Cp - 0.392574Cp^2 + 1.3144876E-04Cp^3$$

$$T(999.51) = 588 \quad T(1090.42) = 1001 \quad T(1132.44) = 1365$$

$$\text{std error est} = 2.0 \qquad \qquad \qquad \text{max error est} = 4.5$$

OXYGEN (Monatomic) 0 100-1500K

$$Cp(T) = 1585.2189 - 1.215663T + 2.1959047E-03T^2 - 1.99642E-06T^3 + 8.9693573E-10T^4 - 1.5832808E-13T^5$$

$$Cp(100) = 1483.70 \quad Cp(800) = 1311.40 \quad Cp(1500) = 1303.03$$

$$\text{std error est} = 2.2 \qquad \qquad \qquad \text{max error est} = 4.5$$

OXYGEN FLUORIDE OF₂ 250-1500K

$$Cp(T) = 332.589 + 2.433234T - 3.634798E-03T^2 + 2.898411E-06T^3 - 1.1968015E-09T^4 + 2.0153116E-13T^5$$

$$Cp(250) = 754.53 \quad Cp(800) = 1012.72 \quad Cp(1500) = 1057.85$$

$$\text{std error est} = 0.6 \qquad \qquad \qquad \text{max error est} = 2.5$$

OXYGEN FLUORIDE (continued)

Note: For T(Cp) calculations, use the iterative procedures discussed in Section 5 and the following eqn: 250-1500K, $C_p(T) = 473.5175767 + 1.433681085T - 1.2241397E-03T^2 + 3.5368257E-07T^3$.

n-PENTANE - Ideal gas C₅H₁₂ 275-755K

$C_p(T) = 272.2797 + 4.8751313T - 7.26261E-05T^2 - 1.3441227E-06T^3$
 $C_p(255) = 1488.43 \quad C_p(500) = 2523.67 \quad C_p(755) = 3333.14$
 std error est = 0.2 max error est = 1.5

$$C_p(T) = \frac{755-1365K}{T} - 3335.717 - 8.6427T + 2.4429916E-02T^2 - 2.47927E-05T^3 + 1.16644237E-08T^4 - 3.12511209E-12T^5$$

$C_p(755) = 3332.45 \quad C_p(1000) = 3859.55 \quad C_p(1365) = 4378.1$
 $\text{std error est} = 0.4 \quad \text{max error est} = 1.5$

$$T(Cp) = -212.8507 + 0.43514236Cp - \frac{1.13646E-04Cp^2}{255-755K} + 2.102165E-08Cp^3$$

$$T(1488.43) = 252 \quad T(2523.67) = 499 \quad T(3333.14) = 754$$

std error est = 0.6 max error est = 2.5
 $T(C_p) = -5111.7 + 4.53933127C_p - \frac{755-1365K}{1.2637957E-03C_p^2} + 1.29008845E-07C_p^3$
 $T(3332.45) = 755 \quad T(3859.55) = 999 \quad T(4378.1) = 1364$
 std error est = 0.6 max error est = 2.5

n-PENTANE - Real gas

PENTANE real gas ~~275-610~~
 $C_p(T) = 568.52265 + 3.2610887T + 2.9780582E-03T^2 - 3.3016552E-06T^3$
 $C_p(275) = 1621.87 \quad C_p(475) = 2435.62 \quad C_p(610) = 2916.51$
 std error est = 1.1 max error est = 2.5

$T(Cp) = -24.41966 + 0.14680646Cp + \frac{275-610K}{2.40140066E-05Cp^2}$
 $T(1621.87) = 277$ $T(2435.62) = 476$ $T(2916.51) = 608$
 std error est = 1.0 max error est = 2.5

1-PENTANOL $\text{CH}_3(\text{CH}_2)_3\text{OH}$ 420-575K

$$\ln[C_p(T)] = 10.279185082 - 1.70935586E-02T + 3.51784187E-05T^2 - 2.23529412E-08T^3$$

Cp(420) = 2098.13 Cp(500) = 2280.35 Cp(575) = 2516.24
****Note: Cp(T) = exp[fctn(T)] max error est = 31.5**

3-PENTANONE $(\text{C}_3\text{H}_7)_2\text{CO}$ 275-1275K

$$Cp(T) = 454.357 + 3.5460727T - 7.37756E-06T^2 - 1.42200623E-06T^3 + 5.2151059E-10T^4$$

3-PENTANONE (continued)

$T(C_p) = 613.076 - 1.234964C_p + \frac{275-1275K}{4}C_p^2 - 3.77839E-07C_p^3$
 $+ 4.8618495E-11C_p^4$
 $T(1402.39) = 276 \quad T(2904.59) = 874 \quad T(3394.43) = 1273$
 $\underline{\text{std error est} = 4.6} \quad \underline{\text{max error est} = 12.5}$

1-PENTENE $\text{CH}_2\text{CH}(\text{CH}_2)_2\text{CH}_3$ 300-1000K

$C_p(T) = -2907.644 + 35.149484T - 0.12403026T^2 + 2.59522805E-04T^3$
 $- 3.0126233E-07T^4 + 1.8150582E-10T^5 - 4.4468884E-14T^6$
 $C_p(300) = 1450.01 \quad C_p(600) = 2583.63 \quad C_p(1000) = 3508.99$
 $\underline{\text{std error est} = 0.7} \quad \underline{\text{max error est} = 2.0}$

$\underline{\text{300-1000K}}$

$T(C_p) = 687.768 - 1.0899882C_p + \frac{300-1000K}{4}C_p^2 - 2.5959466E-07C_p^3$
 $+ 2.9687246E-11C_p^4$
 $T(1450.01) = 300 \quad T(2583.63) = 600 \quad T(3508.99) = 999$
 $\underline{\text{std error est} = 1.1} \quad \underline{\text{max error est} = 2.5}$

1-PENTYNE $\text{HCCCH}_2\text{CH}_2\text{CH}_3$ 300-1500K

$C_p(T) = 728.51 + 0.945078T + 1.1769974E-02T^2 - 2.4194313E-05T^3$
 $+ 2.2017637E-08T^4 - 9.7690847E-12T^5 + 1.7071486E-15T^6$
 $C_p(300) = 1573.93 \quad C_p(600) = 2480.27 \quad C_p(1500) = 3698.55$
 $\underline{\text{std error est} = 2.3} \quad \underline{\text{max error est} = 5.5}$

$\underline{\text{300-1500K}}$

$T(C_p) = 1238.15 - 2.163448C_p + \frac{300-1500K}{4}C_p^2 - 4.685943E-07C_p^3$
 $+ 5.38393765E-11C_p^4$
 $T(1573.93) = 301 \quad T(2480.27) = 604 \quad T(3698.55) = 1493$
 $\underline{\text{std error est} = 4.9} \quad \underline{\text{max error est} = 10.5}$

2-PENTYNE $\text{CH}_3\text{CCH}_2\text{CH}_3$ 300-1500K

$C_p(T) = 452.2996 + 2.3209779T + 5.95716E-03T^2 - 1.31102E-05T^3$
 $+ 1.156122E-08T^4 - 4.958557E-12T^5 + 8.4360724E-16T^6$
 $C_p(300) = 1412.97 \quad C_p(800) = 2741.04 \quad C_p(1500) = 3574.30$
 $\underline{\text{std error est} = 2.2} \quad \underline{\text{max error est} = 4.5}$

$\underline{\text{300-1500K}}$

$T(C_p) = 921.43 - 1.691162C_p + \frac{300-1500K}{4}C_p^2 - 4.3702767E-07C_p^3$
 $+ 5.350453E-11C_p^4$
 $T(1412.97) = 300 \quad T(2741.04) = 799 \quad T(3574.30) = 1498$
 $\underline{\text{std error est} = 3.9} \quad \underline{\text{max error est} = 7.5}$

PHOSGENE COCl_2 100-1500K

$C_p(T) = 191.11 + 2.065565T - 3.2659378E-03T^2 + 2.8264054E-06T^3$
 $- 1.2613311E-09T^4 + 2.2603022E-13T^5$

PHOSGENE (continued)

$C_p(100) = 367.71$ $C_p(800) = 757.91$ $C_p(1500) = 811.14$
 $\underline{\underline{std\ error\ est = 1.8}}$ $\underline{\underline{max\ error\ est = 3.5}}$

PHOSPHINE PH_3 100-1500K

$$C_p(T) = 1105.46 - 2.30246882T + 1.2040496E-02T^2 - 1.9018E-05T^3 \\ + 1.541445E-08T^4 - 6.4490826E-12T^5 + 1.0993473E-15T^6$$

$C_p(100) = 978.08$ $C_p(800) = 1720.90$ $C_p(1500) = 2142.31$
 $\underline{\underline{std\ error\ est = 1.3}}$ $\underline{\underline{max\ error\ est = 2.5}}$

PHOSPHINE, TRIDEUTERATED PD_3 300-1000K

$$C_p(T) = 577.57 + 1.8502044T + 7.1804343E-04T^2 - 2.132996E-06T^3 \\ + 9.1328895E-10T^4$$

$C_p(300) = 1147.06$ $C_p(700) = 1712.22$ $C_p(1000) = 1926.11$
 $\underline{\underline{std\ error\ est = 0.4}}$ $\underline{\underline{max\ error\ est = 1.5}}$

$$T(C_p) = 4259.23 - 12.773886C_p + \frac{1.4525346E-02}{4}C_p^2 - 7.085359E-06C_p^3 \\ + 1.3141044E-09C_p^4$$

$T(1147.06) = 300$ $T(1712.22) = 700$ $T(1926.11) = 1000$
 $\underline{\underline{std\ error\ est = 0.9}}$ $\underline{\underline{max\ error\ est = 3.5}}$

PHOSPHORUS TRICHLORIDE PCl_3 100-1500K

$$C_p(T) = 118.82 + 2.8526816T - 7.620737E-03T^2 + 1.10669999E-05T^3 \\ - 8.9651026E-09T^4 + 3.799535E-12T^5 - 6.55658E-16T^6$$

$C_p(100) = 338.09$ $C_p(800) = 591.05$ $C_p(1500) = 600.84$
 $\underline{\underline{std\ error\ est = 0.6}}$ $\underline{\underline{max\ error\ est = 1.5}}$

PHOSPHORUS TRIFLUORIDE PF_3 100-1500K

$$C_p(T) = 250.76 + 1.7158179T - 4.21548E-04T^2 - 3.5547345E-06T^3 \\ + 5.2965343E-09T^4 - 3.00115347E-12T^5 + 6.166475E-16T^6$$

$C_p(100) = 415.07$ $C_p(800) = 881.29$ $C_p(1500) = 926.47$
 $\underline{\underline{std\ error\ est = 1.8}}$ $\underline{\underline{max\ error\ est = 4.5}}$

PROPADIENE $\text{C}(\text{CH}_2)_2$ 275-1500K

$$C_p(T) = 252.095 + 4.5469778T - 4.231012E-04T^2 - 5.3604454E-06T^3 \\ + 6.62186899E-09T^4 - 3.3478109E-12T^5 + 6.3370948E-16T^6$$

$C_p(275) = 1391.92$ $C_p(800) = 2655.77$ $C_p(1500) = 3348.20$
 $\underline{\underline{std\ error\ est = 0.9}}$ $\underline{\underline{max\ error\ est = 3.5}}$

275-1500K

$$T(C_p) = 1271.52 - 2.4411838C_p + \frac{1.9691654E-03}{4}C_p^2 - 6.3636372E-07C_p^3 \\ + 8.1224744E-11C_p^4$$

$T(1391.92) = 278$ $T(2655.77) = 798$ $T(3348.20) = 1495$

PROPADIENE (continued)

- std error est = 3.3 max error est = 7.5

PROPANE - Ideal gas C_3H_8 275-755K

$$Cp(T) = 84.1607 + 5.7701407T - 1.292127E-03T^2 - 6.9945925E-07T^3$$

$$Cp(275) = 1558.69 \quad Cp(500) = 2558.77 \quad Cp(755) = 3403.05$$

$$std\ error\ est = 0.2 \quad max\ error\ est = 1.5$$

755-1365K

$$Cp(T) = 3474.56 - 9.4956207T + 2.643558E-02T^2 - 2.6640384E-05T^3$$

$$+ 1.2466175E-08T^4 - 2.271073E-12T^5$$

$$Cp(755) = 3402.59 \quad Cp(1000) = 3969.24 \quad Cp(1365) = 4529.56$$

$$std\ error\ est = 0.4 \quad max\ error\ est = 1.5$$

275-755K

$$T(Cp) = -134.47 + 0.349Cp - 8.1104732E-05Cp^2 + 1.623344E-08Cp^3$$

$$T(1558.69) = 274 \quad T(2558.77) = 499 \quad T(3403.05) = 754$$

$$std\ error\ est = 0.6 \quad max\ error\ est = 2.5$$

755-1365K

$$T(Cp) = -4331.0 + 3.78505Cp - 1.0204888E-03Cp^2 + 1.02092847E-07Cp^3$$

$$T(3402.59) = 755 \quad T(3969.24) = 999 \quad T(4529.56) = 1364$$

- std error est = 0.6 max error est = 2.5

CYCLOPROPANE C_3H_8 100-1000K

$$Cp(T) = 1304.37 - 9.76052T + 5.6216148E-02T^2 - 9.9085315E-05T^3$$

$$+ 7.8256763E-08T^4 - 2.34147557E-11T^5$$

$$Cp(100) = 798.99 \quad Cp(600) = 2604.79 \quad Cp(1000) = 3516.69$$

- std error est = 3.3 max error est = 8.5

1,2-PROPANEDIOL $CH_3CHOHCH_2OH$ 275-775K

$$Cp(T) = 840.077 + 1.432479T + 7.47762E-03T^2 - 1.398118E-05T^3$$

$$+ 7.503585E-09T^4$$

$$Cp(275) = 1551.65 \quad Cp(525) = 2200.05 \quad Cp(775) = 2640.29$$

$$std\ error\ est = 3.4 \quad max\ error\ est = 7.5$$

275-775K

$$T(Cp) = -170.21 + 0.384686Cp - 1.377934E-04Cp^2 + 4.859613E-08Cp^3$$

$$T(1551.65) = 276 \quad T(2200.05) = 527 \quad T(2640.29) = 779$$

- std error est = 2.1 max error est = 6.5

1-PROPANOL $CH_3(CH_2)_2OH$ 275-1500K

$$Cp(T) = -18.073 + 4.897967T + 4.1591909E-03T^2 - 1.714072E-05T^3$$

$$+ 1.9134617E-08T^4 - 9.587348E-12T^5 + 1.8328355E-15T^6$$

$$Cp(275) = 1382.08 \quad Cp(800) = 2962.56 \quad Cp(1500) = 3779.34$$

$$std\ error\ est = 2.2 \quad max\ error\ est = 4.5$$

275-1500K

$$T(Cp) = 805.72 - 1.316275Cp + 1.03367336E-03Cp^2 - 3.1066055E-07Cp^3$$

$$+ 3.7595022E-11Cp^4$$

1-PROPANOL (continued)

T(1382.08) = 278 T(2962.56) = 797 T(3779.34) = 1495
std error est = 4.0 max error est = 9.5

2-PROPANOL $(\text{CH}_3)_2\text{CHOH}$ 275-1500K

$$\begin{aligned} \text{Cp}(T) = & 281.08 + 3.55930603T + 5.60782535E-03T^2 - 1.592439E-05T^3 \\ & + 1.567946E-08T^4 - 7.2127354E-12T^5 + 1.289756E-15T^6 \end{aligned}$$

Cp(275) = 1431.69 Cp(800) = 2961.18 Cp(1500) = 3789.51
std error est = 2.5 max error est = 6.5

275-1500K

$$\begin{aligned} \text{T(Cp)} = & 712.46 - 1.195778\text{Cp} + 9.704307E-04\text{Cp}^2 - 2.9394792E-07\text{Cp}^3 \\ & + 3.576185E-11\text{Cp}^4 \end{aligned}$$

T(1431.69) = 277 T(2961.18) = 798 T(3789.51) = 1495
std error est = 3.3 max error est = 6.5

PROPYLBENZENE $\text{C}_6\text{H}_5(\text{CH}_2)_2\text{CH}_3$ 300-1500K

$$\begin{aligned} \text{Cp}(T) = & 156.805 + 2.42815T + 9.353183E-03T^2 - 2.149015E-05T^3 \\ & + 1.9780312E-08T^4 - 8.6963805E-12T^5 + 1.499592E-15T^6 \end{aligned}$$

Cp(300) = 1286.98 Cp(800) = 2727.9 Cp(1500) = 3495.42
std error est = 1.8 max error est = 4.0

300-1500K

$$\begin{aligned} \text{T(Cp)} = & 788.38 - 1.415034\text{Cp} + 1.254462E-03\text{Cp}^2 - 4.2097165E-07\text{Cp}^3 \\ & + 5.5624451E-11\text{Cp}^4 \end{aligned}$$

T(1286.98) = 300 T(2727.9) = 798 T(3495.42) = 1494
std error est = 3.9 max error est = 7.5

PROPYL ETHER $[\text{CH}_3(\text{CH}_2)_2]_2\text{O}$ 275-1275K

$$\begin{aligned} \text{Cp}(T) = & 2220.965 - 15.85878T + 8.362134E-02T^2 - 1.752393E-04T^3 \\ & + 1.89973E-07T^4 - 1.0442973E-10T^5 + 2.2914465E-14T^6 \end{aligned}$$

Cp(275) = 1471.38 Cp(775) = 2885.54 Cp(1275) = 3333.43
std error est = 9.0 max error est = 21.5

PROPYNE CH_3CCH 275-1500K

$$\begin{aligned} \text{Cp}(T) = & 296.204 + 5.18992T - 4.4112215E-03T^2 + 2.621706E-06T^3 \\ & - 9.5357975E-10T^4 + 1.5122198E-13T^5 \end{aligned}$$

Cp(275) = 1439.14 Cp(800) = 2626.24 Cp(1500) = 3324.94
std error est = 0.7 max error est = 3.5

275-1500K

$$\begin{aligned} \text{T(Cp)} = & 1475.3 - 2.85557\text{Cp} + 2.245565E-03\text{Cp}^2 - 7.110777E-07\text{Cp}^3 \\ & + 8.859352E-11\text{Cp}^4 \end{aligned}$$

T(1439.14) = 277 T(2626.24) = 798 T(3324.94) = 1496
std error est = 2.7 max error est = 7.5

SILANE SiH_4 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 1250.39 - 4.4063697T + 0.02678T^2 - 4.8775018E-05T^3 \\ & + 4.4327926E-08T^4 - 2.0245577E-11T^5 + 3.687426E-15T^6 \\ \text{Cp}(100) = & 1033.1 \quad \text{Cp}(800) = 2390.97 \quad \text{Cp}(1500) = 2952.51 \\ \text{std error est} = & 5.8 \quad \text{max error est} = 20.5 \end{aligned}$$

SILICON TETRACHLORIDE SiCl_4 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 112.78 + 2.865988T - 7.278228E-03T^2 + 1.0156921E-05T^3 \\ & - 7.960333E-09T^4 + 3.27887075E-12T^5 - 5.517042E-16T^6 \\ \text{Cp}(100) = & 335.99 \quad \text{Cp}(800) = 617.09 \quad \text{Cp}(1500) = 630.84 \\ \text{std error est} = & 1.0 \quad \text{max error est} = 2.5 \end{aligned}$$

SILICON TETRAFLUORIDE SiF_4 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 142.66 + 3.045967T - 5.205945E-03T^2 + 5.425593E-06T^3 \\ & - 3.534804E-09T^4 + 1.32511825E-12T^5 - 2.1643323E-16T^6 \\ \text{Cp}(100) = & 400.28 \quad \text{Cp}(800) = 955.15 \quad \text{Cp}(1500) = 1011.97 \\ \text{std error est} = & 0.7 \quad \text{max error est} = 1.5 \end{aligned}$$

STYRENE $\text{C}_6\text{H}_5\text{CHCH}_2$ 275-1500K

$$\begin{aligned} \text{Cp}(T) = & -126.7 + 4.27917184T + 2.927387E-03T^2 - 1.2277425E-05T^3 \\ & + 1.2935809E-08T^4 - 6.1243779E-12T^5 + 1.11436976E-15T^6 \\ \text{Cp}(275) = & 1080.96 \quad \text{Cp}(800) = 2467.92 \quad \text{Cp}(1500) = 3116.28 \\ \text{std error est} = & 1.1 \quad \text{max error est} = 2.5 \end{aligned}$$

275-1500K

$$\begin{aligned} \text{T(Cp)} = & 913.36 - 1.888481\text{Cp} + 1.8311187E-03\text{Cp}^2 - 6.899175E-07\text{Cp}^3 \\ & + 1.01386298E-10\text{Cp}^4 \\ \text{T}(1080.96) = & 279 \quad \text{T}(2467.92) = 796 \quad \text{T}(3116.28) = 1493 \\ \text{std error est} = & 4.5 \quad \text{max error est} = 10.5 \end{aligned}$$

SULFUR S_2 275-1500K

$$\begin{aligned} \text{Cp}(T) = & 376.86 + 0.6300876T - 7.88127E-04T^2 + 4.5750016E-07T^3 \\ & - 1.0076704E-10T^4 \\ \text{Cp}(275) = & 499.46 \quad \text{Cp}(800) = 569.24 \quad \text{Cp}(1500) = 580.95 \\ \text{std error est} = & 0.5 \quad \text{max error est} = 2.5 \end{aligned}$$

Note: For $\text{T}(\text{Cp})$ calculations, use the iterative procedures discussed in Section 5 and the following eqn: 275-1500K, $\text{Cp}(T) = 3409.44875 + 0.421901486T - 3.57102338E-04T^2 + 1.02449694E-07T$

SULFUR (Monatomic) S 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 504.485 + 2.3393178T - 8.5202771E-03T^2 + 1.43794546E-05T^3 \\ & - 1.26931826E-08T^4 + 5.67465485E-12T^5 - 1.0136105E-15T^6 \\ \text{Cp}(100) = & 666.38 \quad \text{Cp}(800) = 679.87 \quad \text{Cp}(1500) = 660.51 \\ \text{std error est} = & 1.2 \quad \text{max error est} = 3.0 \end{aligned}$$

SULFUR DICHLORIDE SCl_2 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 239.65 + 1.59183756T - 3.52713E-03T^2 + 4.2688109E-06T^3 \\ & - 2.9106702E-09T^4 + 1.0505776E-12T^5 - 1.5627007E-16T^6 \end{aligned}$$

$$\text{Cp}(100) = 367.55 \quad \text{Cp}(800) = 552.47 \quad \text{Cp}(1500) = 561.14$$

- std error est = 0.9 - - - - - max error est = 2.5

SULFUR DIFLUORIDE SF_2 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 446.1812 - 0.070297366T + 4.760524E-03T^2 - 1.189425E-05T^3 \\ & + 1.2720916E-08T^4 - 6.4083936E-12T^5 + 1.2442913E-15T^6 \end{aligned}$$

$$\text{Cp}(100) = 476.07 \quad \text{Cp}(800) = 783.59 \quad \text{Cp}(1500) = 817.97$$

- std error est = 3.5 - - - - - max error est = 8.0

SULFUR DIOXIDE SO_2 300-1365K

Ideal gas

$$\begin{aligned} \text{Cp}(T) = & 432.805 + 0.5994156T + 4.593367E-04T^2 - 1.433024E-06T^3 \\ & + 1.0409341E-09T^4 - 2.5313735E-13T^5 \end{aligned}$$

$$\text{Cp}(300) = 623.09 \quad \text{Cp}(700) = 793.33 \quad \text{Cp}(1365) = 876.40$$

std error est = 0.3 max error est = 1.5

300-1365K

$$\begin{aligned} T(\text{Cp}) = & 155222.71 - 877.595265\text{Cp} + 1.857197245\text{Cp}^2 - 1.7428909E-03\text{Cp}^3 \\ & + 6.1359879E-07\text{Cp}^4 \end{aligned}$$

$$T(623.09) = 309 \quad T(793.33) = 696 \quad T(876.40) = 1342$$

- std error est = 5.5 - - - - - max error est = 23.5

SULFUR HEXAFLUORIDE SF_6 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 24.233 + 2.33532T + 1.4344428E-03T^2 - 1.05440664E-05T^3 \\ & + 1.3847595E-08T^4 - 7.6376433E-12T^5 + 1.56118585E-15T^6 \end{aligned}$$

$$\text{Cp}(100) = 262.88 \quad \text{Cp}(800) = 990.5 \quad \text{Cp}(1500) = 1056.46$$

- std error est = 5.7 - - - - - max error est = 11.5

SULFUR MONOCHLORIDE S_2Cl_2 100-1500K

$$\begin{aligned} \text{Cp}(T) = & 150.63 + 2.756806T - 7.3955367E-03T^2 + 1.07461656E-05T^3 \\ & - 8.69281614E-09T^4 + 3.6742817E-12T^5 - 6.31809797E-16T^6 \end{aligned}$$

$$\text{Cp}(100) = 362.27 \quad \text{Cp}(800) = 602.75 \quad \text{Cp}(1500) = 611.68$$

- std error est = 0.9 - - - - - max error est = 2.5

SULFUR MONOXIDE SO 300-1500K

$$\text{Cp}(T) = 498.98 + 0.54531131T - 3.97417036E-04T^2 + 1.0243734E-07T^3$$

$$\text{Cp}(300) = 629.57 \quad \text{Cp}(900) = 742.53 \quad \text{Cp}(1500) = 768.48$$

std error est = 0.7 max error est = 2.0

300-1500K

$$\begin{aligned} T(\text{Cp}) = & 2673548.1 - 15732.3334\text{Cp} + 34.6862568\text{Cp}^2 - 3.3963896E-02\text{Cp}^3 \\ & + 1.24657038E-05\text{Cp}^4 \end{aligned}$$

$$T(629.57) = 301 \quad T(742.53) = 902 \quad T(768.48) = 1513$$

SULFUR MONOXIDE (continued)

- std error est = 2.5 max error est = 15.5

SULFUR TETRAFLUORIDE SF₄ 100-1500K

$$\ln[Cp(T)] = 5.4481069265 + 5.31628197E-03T - 7.63297357E-06T^2 \\ + 4.87033913E-09T^3 - 1.14651855E-12T^4$$

$$Cp(200) = 514.49 \quad Cp(800) = 934.52 \quad Cp(1500) = 974.07$$

- **Note: Cp(T) = exp[fctn(T)] max error est = 15.5

SULFUR TRIOXIDE SO₃ 100-1500K

$$Cp(T) = 332.45 + 0.76715644T + 2.18883267E-03T^2 - 6.4464146E-06T^3 \\ + 6.8053136E-09T^4 - 3.3274957E-12T^5 + 6.2860794E-16T^6$$

$$Cp(100) = 425.26 \quad Cp(800) = 908.35 \quad Cp(1500) = 995.38$$

- std error est = 1.4 max error est = 3.5

SULFURYL FLUORIDE SO₂F₂ 100-1500K

$$Cp(T) = 188.38 + 1.51815532T + 1.6848848E-03T^2 - 8.08750268E-06T^3 \\ + 9.88024136E-09T^4 - 5.25778454E-12T^5 + 1.0506054E-15T^6$$

$$Cp(100) = 349.89 \quad Cp(800) = 939.92 \quad Cp(1500) = 1020.75$$

- std error est = 3.2 max error est = 7.5

THIONYL CHLORIDE SOC₁₂ 100-1500K

$$Cp(T) = 126.39 + 3.01522T - 8.0321113E-03T^2 + 1.2067313E-05T^3 \\ - 1.01854131E-08T^4 + 4.48266475E-12T^5 - 7.98302653E-16T^6$$

$$Cp(100) = 358.68 \quad Cp(800) = 664.14 \quad Cp(1500) = 687.57$$

- std error est = 1.4 max error est = 3.5

THIONYL FLUORIDE SOF₂ 100-1500K

$$Cp(T) = 252.57 + 1.591359T + 9.12985723E-05T^2 - 4.47083245E-06T^3 \\ + 6.1962479E-09T^4 - 3.45812419E-12T^5 + 7.09108083E-16T^6$$

$$Cp(100) = 408.73 \quad Cp(800) = 885.74 \quad Cp(1500) = 941.53$$

- std error est = 2.3 max error est = 5.5

THIOPHOSGENE CSCl₂ 275-1000K

$$Cp(T) = 59.14 + 3.3998836T - 8.5876389E-03T^2 + 1.1794626E-05T^3 \\ - 8.30715093E-09T^4 + 2.33820883E-12T^5$$

$$Cp(275) = 546.13 \quad Cp(600) = 660.37 \quad Cp(1000) = 697.07$$

std error est = 0.7 max error est = 2.5

275-1000K

$$T(Cp) = 488250.36 - 3272.97043Cp + 8.22103684Cp^2 - 9.17008593E-03Cp^3 \\ + 3.83549875E-06Cp^4$$

$$T(546.13) = 277 \quad T(660.37) = 589 \quad T(697.07) = 989$$

- std error est = 9.4 max error est = 21.5

TOLUENE C₇H₈

275-755K

Ideal gas

$$Cp(T) = -310.29 + 5.640685T - 2.81410224E-03T^2 + 2.4913887E-07T^3$$

$$Cp(275) = 1033.26 \quad Cp(500) = 1837.67 \quad Cp(755) = 2451.54$$

$$std\ error\ est = 0.2 \quad max\ error\ est = 2.0$$

755-1365K

$$Cp(T) = 109.89 + 4.64889983T - 2.404749E-03T^2 + 4.70371704E-07T^3$$

$$Cp(755) = 2451.48 \quad Cp(1000) = 2824.41 \quad Cp(1365) = 3171.35$$

$$std\ error\ est = 0.2 \quad max\ error\ est = 2.0$$

275-755K

$$T(Cp) = -62.5 + 0.441587267Cp - 1.62355359E-04Cp^2 + 4.8116433E-08Cp^3$$

$$T(1033.26) = 274 \quad T(1837.67) = 499 \quad T(2451.54) = 753$$

$$std\ error\ est = 0.7 \quad max\ error\ est = 3.0$$

755-1365K

$$T(Cp) = -6732.5 + 8.1967182Cp - 3.1808569E-03Cp^2 + 4.4184319E-07Cp^3$$

$$T(2451.48) = 755 \quad T(2824.41) = 999 \quad T(3171.35) = 1364$$

$$std\ error\ est = 0.9 \quad max\ error\ est = 2.5$$

TOLUENE - Real gas

300-610K

$$Cp(T) = 8.203797 + 4.000876T + 1.11409614E-04T^2 - 1.5192015E-06T^3$$

$$Cp(300) = 1177.48 \quad Cp(450) = 1692.72 \quad Cp(610) = 2145.36$$

$$std\ error\ est = 1.2 \quad max\ error\ est = 3.0$$

300-610K

$$T(Cp) = -91.3 + 0.44221698Cp - 1.4179088E-04Cp^2 + 4.099999E-08Cp^3$$

$$T(1177.48) = 300 \quad T(1692.72) = 450 \quad T(2145.36) = 610$$

$$std\ error\ est = 0.6 \quad max\ error\ est = 2.5$$

1,1,1-TRICHLOROETHANE

CH₃CCl₃ 300-600K

$$Cp(T) = 558.306\exp(0.0011T)$$

$$Cp(300) = 776.59 \quad Cp(450) = 915.9 \quad Cp(600) = 1080.21$$

**Note: The accuracy of this fit is within 5.0% of the reference source values. The estimated maximum error is 45.

TRICHLOROFLUORO-

CCl₃F 90-700K (FREON-11)

METHANE - Ideal gas

$$Cp(T) = 88.42 + 2.6878447T - 4.66910945E-03T^2 + 3.96538806E-06T^3$$

$$- 1.311654E-09T^4$$

$$Cp(90) = 295.31 \quad Cp(450) = 660.02 \quad Cp(700) = 727.25$$

$$std\ error\ est = 0.3 \quad max\ error\ est = 2.5$$

700-1365K

$$Cp(T) = 398.846 + 0.85444834T - 6.7934387E-04T^2 + 1.8385308E-07T^3$$

$$Cp(700) = 727.14 \quad Cp(1000) = 757.8 \quad Cp(1365) = 766.99$$

$$std\ error\ est = 0.2 \quad max\ error\ est = 2.5$$

TRICHLOROFLUOROMETHANE (FREON-11) (continued)

90-700K

$$T(Cp) = 1858.9 - 17.09586Cp + 5.92007E-02Cp^2 - 8.71182475E-05Cp^3 \\ + 4.813565E-08Cp^4$$

T(295.31) = 96 T(660.02) = 451 T(727.25) = 693
 std error est = 3.8 max error est = 9.5

Note: For T(Cp) calculations from 700-1365K, use the iterative procedures discussed in Section 5 and the following equations:
 $700-1365K, Cp(T) = 573.5800054 + 0.306189477T - 1.21913823E-04T^2.$

TRICHLOROTRIFLUORO- $C_2Cl_3F_3$ 320-465K

ETHANE (FREON-113)

$$Cp(T) = 953.33 - 4.1752099T + 1.48443126E-02T^2 - 1.4511695E-05T^3$$

Cp(320) = 661.80 Cp(425) = 746.12 Cp(465) = 762.5
 std error est = 0.1 max error est = 1.5

$$T(Cp) = -39428.5 + 169.22394Cp - 0.2413860737Cp^2 + 1.1549402E-04Cp^3$$

T(661.80) = 318 T(746.12) = 426 T(762.5) = 462
 std error est = 1.7 max error est = 4.5

TRICHLOROSILANE $SiHCl_3$ 100-1000K

$$Cp(T) = 163.34 + 2.096026T - 3.3286844E-03T^2 + 2.57996254E-06T^3 \\ - 7.76498622E-10T^4$$

Cp(100) = 342.16 Cp(600) = 679.27 Cp(1000) = 734.15
 std error est = 1.5 max error est = 3.5

$$T(Cp) = 9037.45 - 76.410239Cp + 0.238723665Cp^2 - 3.24312525E-04Cp^3 \\ + 1.64234225E-07Cp^4$$

T(342.16) = 101 T(679.27) = 602 T(734.15) = 990
 std error est = 8.9 max error est = 15.5

1,1,1-TRICHLORO-2,2,2-TRI- CF_3CCl_3 200-800K
 FLUOROETHANE

$$Cp(T) = 185.89 + 1.4044747T + 2.6500078E-03T^2 - 1.18943003E-05T^3 \\ + 1.45980328E-08T^4 - 6.1337978E-12T^5$$

Cp(200) = 499.02 Cp(500) = 784.54 Cp(800) = 885.02
 std error est = 0.7 max error est = 2.0

$$T(Cp) = 7781.2 - 49.265363Cp + 0.117538654Cp^2 - 1.2291743E-04Cp^3 \\ + 4.8509877E-08Cp^4$$

T(499.02) = 200 T(784.54) = 498 T(885.02) = 798
 std error est = 4.3 max error est = 9.5

1,1,1-TRIFLUOROETHANE CH_3CF_3 100-1500K

1,1,1-TRIFLUOROETHANE (continued)

$C_p(T) = 264.398 + 1.8040847T + 4.17525467E-03T^2 - 1.2539045E-05T^3$
 $+ 1.3278592E-08T^4 - 6.49158273E-12T^5 + 1.2220205E-15T^6$
 $C_p(100) = 475.28 \quad C_p(800) = 1591.93 \quad C_p(1500) = 1892.56$
 $- \underline{\text{std error est}} = 1.7 \quad \underline{\text{max error est}} = 3.5$

TRIFLUOROIODOMETHANE CF_3I 100-1000K

$C_p(T) = 103.14 + 1.255612T - 1.56065E-03T^2 + 9.460232E-07T^3$
 $- 2.27049635E-10T^4$
 $C_p(100) = 214.02 \quad C_p(600) = 469.59 \quad C_p(1000) = 517.08$
 $\underline{\text{std error est}} = 0.4 \quad \underline{\text{max error est}} = 2.0$

Note: For $T(C_p)$ calculations, use the iterative procedures discussed in Section 5 and the following eqn: $100-1000K, C_p(T) = 110.51576796 + 1.161867871T - 1.20896094E-03T^2 + 4.5474783E-07T^3$

TRIMETHYLAMINE $(CH_3)_3N$ 275-1475K

$C_p(T) = 773.274 - 1.34861408T + 2.365832E-02T^2 - 4.5452006E-05T^3$
 $+ 4.1145841E-08T^4 - 1.84648686E-11T^5 + 3.29518026E-15T^6$
 $C_p(275) = 1454.01 \quad C_p(875) = 3384.35 \quad C_p(1475) = 4173.36$
 $\underline{\text{std error est}} = 2.1 \quad \underline{\text{max error est}} = 5.5$

$\underline{\text{275-1475K}}$
 $T(C_p) = 430.45 - 0.63430825C_p + 5.6407771E-04C_p^2 - 1.6640782E-07C_p^3$
 $+ 1.9643825E-11C_p^4$
 $T(1454.01) = 277 \quad T(3384.35) = 871 \quad T(4173.36) = 1471$
 $\underline{\text{std error est}} = 3.4 \quad \underline{\text{max error est}} = 7.5$

2,3,4-TRIMETHYL- $[(CH_3)_2CH]_2CHCH_3$ 400-520K

PENTANE

$C_p(T) = 686.88 + 3.789T \quad T(C_p) = [C_p - 686.88]/3.789$
There are only three data points in the reference source. The accuracy of this fit cannot be adequately established.

WATER - Ideal gas H_2O 275-1365K

$C_p(T) = 1997.22 - 1.5513626T + 5.4600474E-03T^2 - 7.4448866E-06T^3$
 $+ 5.92340976E-09T^4 - 2.54654038E-12T^5 + 4.50326153E-16T^6$
 $C_p(275) = 1858.75 \quad C_p(800) = 2148.61 \quad C_p(1365) = 2527.54$
 $\underline{\text{std error est}} = 0.6 \quad \underline{\text{max error est}} = 3.5$

$\underline{\text{275-1365K}}$
 $T(C_p) = -138783.1 + 243.21339C_p - 0.1601304C_p^2 + 4.6992596E-05C_p^3$
 $- 5.155188E-09C_p^4$
 $T(1858.75) = 292 \quad T(2148.61) = 798 \quad T(2527.54) = 1360$
 $\underline{\text{std error est}} = 5.0 \quad \underline{\text{max error est}} = 18.5$

WATER - Real gas

375-545K

$$\begin{aligned} Cp(T) = & -9151.27 + 124.55666T - 0.43018315T^2 + 2.5078185E-04T^3 \\ & + 1.51700823E-06T^4 - 3.1440734E-09T^5 + 1.82314019E-12T^6 \\ Cp(375) = & 2041.49 \quad Cp(500) = 1976.29 \quad Cp(545) = 1990.98 \\ \text{std error est} = & 0.5 \quad \text{max error est} = 2.5 \end{aligned}$$

535-1365K

$$\begin{aligned} Cp(T) = & 1855.87 - 0.12328108T + 8.33819257E-04T^2 - 2.7862857E-07T^3 \\ Cp(535) = & 1985.91 \quad Cp(1000) = 2287.78 \quad Cp(1365) = 2532.55 \\ \text{std error est} = & 0.2 \quad \text{max error est} = 1.5 \end{aligned}$$

Note: For T(Cp) calculations between 375-545K, use the iterative procedures discussed in Section and the following egn: 375-545K,
 $Cp(T) = 7288.57944 - 31.60499289T + 6.19666037E-02T^2 - 4.001532E-05T^3$.

535-1365K

$$\begin{aligned} T(Cp) = & -20093.67 + 24.866517Cp - 1.0260634E-02Cp^2 + 1.495574E-06Cp^3 \\ T(1985.91) = & 536 \quad T(2287.78) = 1000 \quad T(2532.55) = 1365 \\ \text{std error est} = & 0.7 \quad \text{max error est} = 3.5 \end{aligned}$$

WATER, DIDEUTERATED D₂O 0-1500K

$$\begin{aligned} Cp(T) = & 1692.39 + 0.531928T + 9.981787E-04T^2 - 1.32271877E-06T^3 \\ & + 6.3221224E-10T^4 - 1.140281E-13T^5 \\ Cp(1) = & 1692.92 \quad Cp(750) = 2267.77 \quad Cp(1500) = 2606.68 \\ \text{std error est} = & 1.5 \quad \text{max error est} = 3.5 \end{aligned}$$

0-1500K

$$\begin{aligned} T(Cp) = & -262435.28 + 620.045026Cp - 0.58727707Cp^2 + 2.7838713E-04Cp^3 \\ & - 6.59628036E-08Cp^4 + 6.2551268E-12Cp^5 \\ T(1692.92) = & 0 \quad T(2267.77) = 753 \quad T(2606.68) = 1499 \\ \text{std error est} = & 1.2 \quad \text{max error est} = 5.5 \end{aligned}$$

XENON - Ideal gas Xe ALL TEMPERATURES

- Cp(T) = 158.416 = constant -----

m-XYLENE C₆H₄(CH₃)₂ 300-1500K

$$\begin{aligned} Cp(T) = & 112.448 + 2.48622T + 8.20559E-03T^2 - 1.897328E-05T^3 \\ & + 1.749458E-08T^4 - 7.7581914E-12T^5 + 1.35754047E-15T^6 \\ Cp(300) = & 1208.38 \quad Cp(800) = 2618.13 \quad Cp(1500) = 3385.32 \\ \text{std error est} = & 1.4 \quad \text{max error est} = 3.5 \end{aligned}$$

300-1500K

$$\begin{aligned} T(Cp) = & 793.3 - 1.4795435Cp + 1.3653586E-03Cp^2 - 4.736549E-07Cp^3 \\ & + 6.4258022E-11Cp^4 \\ T(1208.38) = & 300 \quad T(2618.13) = 798 \quad T(3385.32) = 1495 \\ \text{std error est} = & 3.8 \quad \text{max error est} = 8.5 \end{aligned}$$

o-XYLENE $C_6H_4(CH_3)_2$ 300-1500K

$$Cp(T) = 220.54 + 2.315837T + 8.00889E-03T^2 - 1.8267628E-05T^3 \\ + 1.67967527E-08T^4 - 7.4499897E-12T^5 + 1.30510608E-15T^6$$

$$Cp(300) = 1261.77 \quad Cp(800) = 2626.74 \quad Cp(1500) = 3387.23 \\ \text{std error est} = 1.0 \qquad \qquad \qquad \text{max error est} = 3.5$$

300-1500K

$$T(Cp) = 884.7 - 1.6751046Cp + 1.49528125E-03Cp^2 - 5.09322185E-07Cp^3 \\ + 6.778076E-11Cp^4$$

$$T(1261.77) = 300 \quad T(2626.74) = 798 \quad T(3387.23) = 1495$$

$$- \text{std error est} = 3.7 \quad - \text{max error est} = 8.5$$

p-XYLENE $C_6H_4(CH_3)_2$ 300-1500K

$$Cp(T) = 240.04 + 1.4903657T + 1.0968075E-02T^2 - 2.28936254E-05T^3 \\ + 2.05420776E-08T^4 - 8.9907546E-12T^5 + 1.56029453E-15T^6$$

$$Cp(300) = 1201.83 \quad Cp(800) = 2607.33 \quad Cp(1500) = 3381.23 \\ \text{std error est} = 0.9 \qquad \qquad \qquad \text{max error est} = 3.5$$

300-1500K

$$T(Cp) = -1458.07 + 4.050261Cp - 3.859663E-03Cp^2 + 1.9113335E-06Cp^3 \\ - 4.63203445E-10Cp^4 + 4.53602623E-14Cp^5$$

$$T(1201.83) = 300 \quad T(2607.33) = 801 \quad T(3381.23) = 1499$$

$$- \text{std error est} = 1.5 \quad - \text{max error est} = 4.5$$

APPENDIX B
TABLE B-I
SUMMARY OF CONTENTS

**THERMAL CONDUCTIVITY FOR
 GASEOUS ELEMENTS AND COMPOUNDS**

NAME	FORMULA	APP B PAGE
Acetone	C ₃ H ₆ O	B-1
Acetylene	C ₂ H ₂	B-1
Air	-	B-1
Ammonia	NH ₃	B-1
Argon	Ar	B-2
Benzene	C ₆ H ₆	B-2
Boron Trifluoride	BF ₃	B-2
Bromine	Br ₂	B-3
iso-Butane	i-C ₄ H ₁₀	B-3
n-Butane	n-C ₄ H ₁₀	B-3
Carbon Dioxide	CO ₂	B-3
Carbon Monoxide	CO	B-4
Carbon Tetrachloride	CCl ₄	B-4
Chlorine	Cl ₂	B-4
Chlorodifluoromethane (FREON-22)	CHClF ₂	B-5
Chloroform	CHCl ₃	B-5
Chlorotrifluoromethane (FREON-13)	CClF ₃	B-5
n-Decane	C ₁₀ H ₂₂	B-5
Deuterium	D ₂	B-5
Dichlorodifluoromethane (FREON-12)	CCl ₂ F ₂	B-6
Dichlorofluoromethane (FREON-21)	CHCl ₂ F	B-6
Dichlorotetrafluoroethane (FREON-114)	C ₂ Cl ₂ F ₄	B-6
Ethane	C ₂ H ₆	B-6
Ethyl Alcohol	C ₂ H ₅ OH	B-7
Ethyl Ether	C ₄ H ₁₀ O	B-7
Ethylene	C ₂ H ₄	B-7
Fluorine	F ₂	B-7
Helium	He	B-7
n-Heptane	C ₇ H ₁₆	B-8
n-Hexane	C ₆ H ₁₄	B-8
Hydrogen	H ₂	B-8
Hydrogen Chloride	HCl	B-9
Hydrogen Iodide	HI	B-9
Hydrogen Sulfide	H ₂ S	B-10

TABLE B-I
(CONT.)

NAME	FORMULA	APP B PAGE
Krypton	Kr	B-10
Methane	CH ₄	B-10
Methyl Alcohol	CH ₃ OH	B-10
Methyl Chloride	CH ₃ Cl	B-10
Neon	Ne	B-11
Nitric Oxide	NO	B-11
Nitrogen	N ₂	B-11
Nitrogen Peroxide	NO ₂	B-12
Nitrous Oxide	N ₂ O	B-12
n-Nonane	C ₉ H ₂₀	B-12
n-Octane	C ₈ H ₁₈	B-13
Oxygen	O ₂	B-13
n-Pentane	C ₅ H ₁₂	B-13
Propane	C ₃ H ₈	B-13
Radon	Rn	B-14
Sulfur Dioxide	SO ₂	B-14
Toluene	C ₇ H ₈	B-14
Trichlorofluoromethane (FREON-11)	CCl ₃ F	B-14
Trichlorotrifluoroethane (FREON-113)	C ₂ Cl ₃ F ₃	B-15
Water (steam)	H ₂ O	B-15
Xenon	Xe	B-15

APPENDIX B
FORMAT EXAMPLE

The equations presented are for gaseous Acetylene

The polynomial equation to calculate the thermal conductivity (k) in W/m K as a function of temperature (Kelvin)

	Formula	Valid temperature range
-ACETYLENE	C_2H_2	200-650K

$$k(T) = -8.5510082E-02 + 1.461749E-03T - 9.4040526E-06T^2 + 3.242075E-08T^3 - 5.91795705E-11T^4 + 5.4937859E-14T^5 - 2.04661826E-17T^6$$

$$k(200) = 0.0116 \quad k(450) = 0.0394 \quad k(650) = 0.0619$$

$$std\ error\ est = 6.3E-05 \quad max\ error\ est = 7E-04$$

$$T(k) = \frac{200-650K}{58.2453 + 13908.7532k - 151692.6999k^2 + 1329757.4619k^3}$$

$$T(0.0116) = 201 \quad T(0.0394) = 452 \quad T(0.0619) = 653$$

$$std\ error\ est = 1.7 \quad max\ error\ est = 3.5$$

standard (or average) error estimate is ± 1.7 degrees Kelvin

The polynomial equation to calculate temperature (Kelvin) as a function of thermal conductivity in W/m K

Using the polynomial presented, the calculated thermal conductivity at 650K is 0.0619 W/m K.

Over the temperature range noted, the maximum error est is $\pm 7E-04$ W/m K.

Using the polynomial presented, the calculated temperature for a given thermal conductivity of 0.0619 W/m K is 653K.

FIGURE B-1

APPENDIX B

THERMAL CONDUCTIVITY FOR
GASEOUS ELEMENTS AND COMPOUNDS

ACETONE

C₃H₆O

280-500K

$$k(T) = -4.11573122E-04 + 4.79793901E-06T + 1.15976849E-07T^2$$

$$k(280) = 0.01002 \quad k(400) = 0.02006 \quad k(500) = 0.03098$$

$$\text{std error est} = 1.8E-05 \quad \text{max error est} = 4.0E-05$$

280-500K

$$T(k) = 136.464 + 15795.28787k - 132356.15338k^2$$

$$T(0.01002) = 281 \quad T(0.02006) = 400 \quad T(0.03098) = 499$$

$$\text{std error est} = 0.7 \quad \text{max error est} = 2.5$$

ACETYLENE

C₂H₂

200-650K

$$k(T) = -8.5510082E-02 + 1.461749E-03T - 9.4040526E-06T^2 \\ + 3.242075E-08T^3 - 5.91795705E-11T^4 + 5.4937859E-14T^5$$

$$- 2.04661826E-17T^6$$

$$k(200) = 0.0116 \quad k(450) = .0394 \quad k(650) = 0.0619$$

$$\text{std error est} = 6.3E-05 \quad \text{max error est} = 7E-04$$

200-650K

$$T(k) = 58.2453 + 13908.7532k - 151692.6999k^2 + 1329757.4619k^3$$

$$T(0.0116) = 201 \quad T(0.0394) = 452 \quad T(0.0619) = 653$$

$$\text{std error est} = 1.7 \quad \text{max error est} = 3.5$$

AIR

100-1500K

$$k(T) = -2.276501E-03 + 1.2598485E-04T - 1.4815235E-07T^2 \\ + 1.73550646E-10T^3 - 1.066657E-13T^4 + 2.47663035E-17T^5$$

$$k(100) = 9.0E-02 \quad k(800) = 0.0570 \quad k(1500) = 0.0872$$

$$\text{std error est} = 1.2E-04 \quad \text{max error est} = 2.5E-04$$

100-1500K

$$T(k) = -21.25887 + 12111.0665k - 2060.85234k^2 + 726814.383446k^3$$

$$T(.009) = 88 \quad T(.0570) = 797 \quad T(.0872) = 1501$$

$$\text{std error est} = 5.0 \quad \text{max error est} = 13.5$$

AMMONIA

NH₃

250-900K

$$k(T) = 3.25332857E-02 - 2.56604839E-04T + 1.19984154E-06T^2 \\ - 1.8411802E-09T^3 + 1.450888E-12T^4 - 4.5463777E-16T^5$$

$$k(250) = 0.0198 \quad k(650) = 0.0733 \quad k(900) = 0.1147$$

$$\text{std error est} = 8.8E-05 \quad \text{max error est} = 2E-04$$

250-900K

$$T(k) = 59.78 + 10975.1917k - 54118.9276k^2 + 195945.59072k^3$$

$$T(.0198) = 257 \quad T(.0733) = 651 \quad T(.1147) = 902$$

$$\text{std error est} = 2.1 \quad \text{max error est} = 4.5$$

ARGON Ar 100-2000K

$$k(T) = -5.2839462E-04 + 7.60706705E-05T - 6.4749393E-08T^2 + 5.41874502E-11T^3 - 3.22024235E-14T^4 + 1.17962552E-17T^5 - 1.86231745E-21T^6$$

$$k(100) = 6.48E-03 \quad k(800) = 0.03682 \quad k(2000) = 0.06921$$

$$\text{std error est} = 4.6E-05 \quad \text{max error est} = 1E-04$$

2000-6000K

$$k(T) = 1.93082997E-02 + 2.51961654E-05T - 1.67510345E-10T^2 + 1.34423776E-14T^3$$

$$k(2000) = 0.06914 \quad k(4000) = 0.11827 \quad k(6000) = 0.16736$$

$$\text{std error est} = 6.2E-05 \quad \text{max error est} = 1E-04$$

6000-10000K

$$k(T) = 9.646322815 - 8.33091359E-03T + 2.95984109E-06T^2 - 5.46353403E-10T^3 + 5.53001474E-14T^4 - 2.90734681E-18T^5 + 6.22212377E-23T^6$$

$$k(6000) = 0.16724 \quad k(8000) = 0.2483 \quad k(10000) = 0.4559$$

$$\text{std error est} = 2.9E-04 \quad \text{max error est} = 4E-04$$

100-2000K

$$T(k) = 6.817 + 13959.6435k + 48739.9133k^2 + 6473513.547817k^3 - 59362842.0531k^4$$

$$T(6.48E-03) = 101 \quad T(0.03682) = 801 \quad T(0.06921) = 1990$$

$$\text{std error est} = 2.5 \quad \text{max error est} = 11$$

2000-6000K

$$T(k) = -806.5 + 40519.97783k + 982.79608093k^2$$

$$T(0.06914) = 2000 \quad T(0.11827) = 4000 \quad T(0.16736) = 6002$$
~~$$\text{std error est} = 2.6 \quad \text{max error est} = 5.0$$~~

BENZENE C₆H₆ 250-600K

$$k(T) = 1.26398664E-02 - 8.09524147E-05T + 2.45397874E-07T^2$$

$$k(250) = 7.74E-03 \quad k(450) = 0.0259 \quad k(600) = 0.05241$$

$$\text{std error est} = 5E-05 \quad \text{max error est} = 1E-04$$

250-600K

$$T(k) = 119.7 + 20654.901668k - 382444.26277k^2 + 3143235.5389k^3$$

$$T(7.74E-03) = 258 \quad T(0.0259) = 453 \quad T(0.05241) = 604$$
~~$$\text{std error est} = 2.9 \quad \text{max error est} = 8.5$$~~

BORON TRIFLUORIDE BF₃ 250-400K

$$k(T) = -0.013508927 + 1.74995767E-04T - 2.88441695E-07T^2 + 2.22936681E-10T^4$$

$$k(250) = 0.0157 \quad k(350) = 0.02196 \quad k(400) = 0.02461$$

$$\text{std error est} = 3.3E-05 \quad \text{max error est} = 1E-04$$

250-400K

$$T(k) = 118.06 + 3008.28162k + 343663.276584k^2$$

$$T(0.0157) = 250 \quad T(0.02196) = 350 \quad T(0.02461) = 400$$
~~$$\text{std error est} = 0.6 \quad \text{max error est} = 1.5$$~~

BROMINE Br_2 250-350K

$k(T) = 1.836200284 - 3.09326519E-02T + 2.07612343E-04T^2$
 $- 6.93057809E-07T^3 + 1.15148285E-09T^4 - 7.61810378E-13T^5$
 $k(250) = 3.8E-03 \quad k(300) = 4.76E-03 \quad k(350) = 5.7E-03$
 $\text{std error est} = 2.1E-05 \quad \text{max error est} = 1E-04$
Note: The pressure dependence between 250-330K has been ignored.
250-350K
 $T(k) = 63.28 + 45883.69957k + 808725.8551494k^2$
 $T(3.8E-03) = 249 \quad T(4.76E-03) = 300 \quad T(5.7E-03) = 351$
~~- std error est = 1.6~~ ~~- max error est = 2.5~~
iso-BUTANE $i\text{-C}_4\text{H}_{10}$ 270-500K
 $k(T) = 7.7275075E-02 - 8.28249983E-04T + 3.48331547E-06T^2$
 $- 5.71799839E-09T^3 + 3.50919304E-12T^4$
 $k(270) = 0.01368 \quad k(400) = 0.02719 \quad k(500) = 0.03855$
 $\text{std error est} = 3.7E-05 \quad \text{max error est} = 1E-04$
270-500K
 $T(k) = 95.54 + 15411.2231k - 219575.79653k^2 + 2403201.4742k^3$
 $T(0.01368) = 271 \quad T(0.02719) = 401 \quad T(0.03855) = 501$
~~- std error est = 0.8~~ ~~- max error est = 2.5~~
n-BUTANE $n\text{-C}_4\text{H}_{10}$ 280-500K
 $k(T) = 3.79912E-03 - 3.38011396E-05T + 3.15886537E-07T^2$
 $- 2.25600514E-10T^3$
 $k(280) = 0.01415 \quad k(400) = 0.02638 \quad k(500) = 0.03767$
 $\text{std error est} = 2.5E-05 \quad \text{max error est} = 1E-04$
280-500K
 $T(k) = 128.42 + 11389.32096k - 41250.42160187k^2$
 $T(0.01415) = 281 \quad T(0.02638) = 400 \quad T(0.03767) = 499$
~~- std error est = 0.7~~ ~~- max error est = 2.0~~
CARBON DIOXIDE CO_2 200-600K
 $k(T) = 2.971488E-03 - 1.33471677E-05T + 3.14443715E-07T^2$
 $- 4.75106178E-10T^3 + 2.68500151E-13T^4$
 $k(200) = 9.51E-03 \quad k(400) = 0.02441 \quad k(600) = 0.04034$
 $\text{std error est} = 2.2E-05 \quad \text{max error est} = 1E-04$
600-1000K
 $k(T) = 6.085375E-02 - 3.63680275E-04T + 1.0134366E-06T^2$
 $- 9.7042356E-10T^3 + 3.27864115E-13T^4$
 $k(600) = 0.04036 \quad k(800) = 0.05595 \quad k(1000) = 0.06805$
 $\text{std error est} = 5.6E-05 \quad \text{max error est} = 1.2E-04$

CARBON DIOXIDE (continued) 1000-1500K
 $k(T) = -4.880854E-02 + 2.05275039E-04T - 1.15912553E-07T^3$
 $+ 2.74425613E-11T^3$
 $k(1000) = 0.0680 \quad k(1250) = 0.08027 \quad k(1500) = 0.09092$
 $\text{std error est} = 4.9E-05 \quad \text{max error est} = 1E-04$

200-600K
 $T(k) = 71.53 + 14079.598772k - 24697.758498k^2$
 $T(9.51E-03) = 203 \quad T(0.02441) = 400 \quad T(0.04034) = 599$
 $\text{std error est} = 1.1 \quad \text{max error est} = 3.5$

600-1000K
 $T(k) = 389.988 - 335.1830848k + 137340.8296339k^2$
 $T(0.04036) = 600 \quad T(0.05595) = 801 \quad T(0.06805) = 1003$
 $\text{std error est} = 1.3 \quad \text{max error est} = 3.5$

1000-1500K
 $T(k) = 438.195 - 2034.64765848k + 151207.6747921k^2$
 $T(0.0680) = 999 \quad T(0.08027) = 1249 \quad T(0.09092) = 1503$
 $\text{std error est} = 1.4 \quad \text{max error est} = 2.5$

CARBON MONOXIDE CO 100-1250K
 $k(T) = -7.41704398E-04 + 9.87435265E-05T - 3.77511167E-08T^2$
 $- 1.99334224E-11T^3 + 3.65528437E-14T^4 - 1.2427179E-17T^5$
 $k(100) = 8.74E-03 \quad k(650) = 0.0471 \quad k(1250) = 0.07608$
 $\text{std error est} = 4E-05 \quad \text{max error est} = 1E-04$

100-1250K
 $T(k) = 12.162 + 8989.653527k + 97279.93110207k^2$
 $T(8.74E-03) = 98 \quad T(0.0471) = 651 \quad T(0.07608) = 1259$
 $\text{std error est} = 3.7 \quad \text{max error est} = 11.0$

CARBON TETRACHLORIDE CC14 250-500K
 $k(T) = 7.8364705E-03 - 7.3966726E-05T + 3.78688851E-07T^2$
 $- 5.67675082E-10T^3 + 2.88855251E-13T^4$
 $k(250) = 5.27E-03 \quad k(400) = 9.9E-03 \quad k(500) = 0.01262$
 $\text{std error est} = 1.1E-05 \quad \text{max error est} = 1E-04$

250-500K
 $T(k) = 108.29 + 25202.5901427k + 442601.9142055k^2$
 $T(5.27E-03) = 253 \quad T(9.9E-03) = 401 \quad T(0.01262) = 497$
 $\text{std error est} = 1.7 \quad \text{max error est} = 5.5$

CHLORINE Cl₂ 240-700K
 $k(T) = -5.6373517E-03 + 7.42811048E-05T - 1.39215986E-07T^2$
 $+ 2.1640488E-10T^3 - 1.2881365E-13T^4$
 $k(240) = 6.74E-03 \quad k(450) = 0.01404 \quad k(700) = 0.02144$
 $\text{std error est} = 4.7E-05 \quad \text{max error est} = 1E-04$

CHLORINE (continued) 240-700K

$$T(k) = 172.043 - 13603.49935k + 5088112.16192k^2 - 265967414.84k^3 + 5207768348.464k^4$$

$$T(6.74E-03) = 240 \quad T(0.01404) = 450 \quad T(0.02144) = 698$$

- std error est = 1.7 - - - - - max_error_est = 5.5

CHLORODIFLUOROMETHANE CHClF_2 250-500K

(FREON-22)

$$k(T) = - 4.0615383E-04 + 1.80841025E-05T + 6.18803419E-08T^2$$

$$k(250) = 7.98E-03 \quad k(400) = 0.01673 \quad k(500) = 0.02411$$

$$\text{std error est} = 2.4E-05 \quad \text{max error est} = 1E-04$$

250-500K

$$T(k) = 85.013 + 22663.6699172k - 228007.2338189k^2$$

$$T(7.98E-03) = 251 \quad T(0.01673) = 400 \quad T(0.02411) = 500$$

- std error est = 0.9 - - - - - max_error_est = 2.5

CHLOROFORM CHCl_3 340-550K

$$k(T) = - 5.860675E-03 + 5.20017788E-05T - 3.8366916E-08T^2 + 3.64052602E-11T^3$$

$$k(340) = 8.82E-03 \quad k(400) = 0.01113 \quad k(550) = 0.01719$$

$$\text{std error est} = 2.5E-05 \quad \text{max error est} = 1E-04$$

340-550K

$$T(k) = 93.34 + 29378.466083k - 162781.2342915k^2$$

$$T(8.82E-03) = 340 \quad T(0.01113) = 400 \quad T(0.01719) = 550$$

- std error est = 0.7 - - - - - max_error_est = 1.5

CHLOROTRIFLUOROMETHANE CClF_3 250-500K

(FREON-13)

$$k(T) = - 5.6286355E-03 + 5.68433027E-05T + 8.34249085E-09T^2$$

$$k(250) = 9.1E-03 \quad k(400) = 0.01844 \quad k(500) = 0.02488$$

$$\text{std error est} = 1.8E-05 \quad \text{max error est} = 1E-04$$

250-500K

$$T(k) = 98.24 + 16976.00664908k - 33295.38946655k^2$$

$$T(9.1E-03) = 250 \quad T(0.01844) = 400 \quad T(0.02488) = 500$$

- std error est = 0.3 - - - - - max_error_est = 1.5

n-DECANE $\text{C}_{10}\text{H}_{22}$ 250-500K

$$k(T) = - 5.88274E-03 + 3.72449646E-05T + 7.55109624E-08T^2$$

$$k(250) = 8.15E-03 \quad k(400) = 0.0211 \quad k(500) = 0.03162$$

$$\text{std error est} = 2.5E-05 \quad \text{max error est} = 1E-04$$

Note: Pressure dependence between 250-440K ignored.

Note: For $T(k)$ calculations, use the iterative procedures discussed in Section 5 and the polynomial presented above. - - -

DEUTERIUM D_2 25-400K

$$k(T) = - 5.698206E-03 + 8.4468815E-04T - 3.02792058E-06T^2$$

$$+ 1.1004468E-08T^3 - 2.1022893E-11T^4 + 1.58585846E-14T^5$$

DEUTERIUM (continued)

$k(25) = 0.01369$ $k(250) = 0.12154$ $k(400) = 0.1762$
 $\text{std error est} = 2.2E-04$ $\text{max error est} = 4E-04$

25-400K

$T(k) = 0.5886 + 1513.21300425k + 4346.0399915k^2$
 $T(0.01369) = 22$ $T(0.12154) = 249$ $T(0.1762) = 402$
 $\text{std error est} = 1.5$ $\text{max error est} = 2.5$

DICHLORODIFLUOROMETHANE CCl_2F_2 250-500K

(FREON-12)

$k(T) = -3.233077E-03 + 3.50076218E-05T + 2.7686436E-08T^2$
 $- 2.30654304E-12T^3$
 $k(250) = 7.21E-03$ $k(400) = 0.01505$ $k(500) = 0.0209$
 $\text{std error est} = 2.6E-05$ $\text{max error est} = 1E-04$

250-500K

$T(k) = 95.995 + 22495.971645k - 152316.4895525k^2$
 $T(7.21E-03) = 250$ $T(0.01505) = 400$ $T(0.0209) = 500$
 $\text{std error est} = 0.5$ $\text{max error est} = 1.5$

DICHLOROFUOROMETHANE CHCl_2F 250-450K

(FREON-21)

$k(T) = -3.70498999E-03 + 5.72092142E-05T - 1.13430816E-07T^2$
 $+ 1.98784186E-10T^3$
 $k(250) = 6.61E-03$ $k(350) = 0.01095$ $k(450) = 0.01718$
 $\text{std error est} = 3.9E-05$ $\text{max error est} = 1E-04$

250-450K

$T(k) = 52.34 + 34343.090676k - 655593.6727497k^2$
 $T(6.61E-03) = 251$ $T(0.01095) = 350$ $T(0.01718) = 449$
 $\text{std error est} = 0.9$ $\text{max error est} = 2.0$

DICHLOROTETRAFLUOROETHANE $\text{C}_2\text{Cl}_2\text{F}_4$ 250-500K

(FREON-114)

$k(T) = 1.5549359E-02 - 7.41226495E-05T + 1.96794871E-07T^2$
 $k(250) = 9.32E-03$ $k(400) = 0.01739$ $k(500) = 0.02769$
 $\text{std error est} = 2.6E-05$ $\text{max error est} = 1E-04$

250-500K

$T(k) = -127.377 + 58481.31774k - 2155849.717k^2 + 31248863.5628k^3$
 $T(9.32E-03) = 256$ $T(0.01739) = 402$ $T(0.02769) = 502$
 $\text{std error est} = 2.5$ $\text{max error est} = 6.5$

ETHANE C_2H_6 200-1000K

$k(T) = -3.83815197E-02 + 5.47282126E-04T - 2.80760648E-06T^2$
 $+ 8.74854603E-09T^3 - 1.369896E-11T^4 + 1.05765043E-14T^5$
 $- 3.16347435E-18T^6$
 $k(200) = 0.01002$ $k(600) = 0.06838$ $k(1000) = 0.16391$
 $\text{std error est} = 1.9E-04$ $\text{max error est} = 3E-04$

200-1000K

$T(k) = 128.505 + 8110.832388k - 17342.93335k^2$
 $T(0.01002) = 208$ $T(0.06838) = 602$ $T(0.16391) = 992$

ETHYL ALCOHOL C₂H₅OH 250-500K

k(T) = - 2.46663E-02 + 1.5589255E-04T - 8.22954822E-08T²
k(250) = 9.17E-03 k(400) = 0.02453 k(500) = 0.03271
std error est = 2.8E-05 max error est = 1E-04

Note: Pressure dependence between 250-350K ignored.

250-500K

T(k) = 183.774 + 6437.651482775k + 97730.4282729k²
T(9.17E-03) = 251 T(0.02453) = 400 T(0.03271) = 499
std error est = 0.7 max error est = 2.0

ETHYL ETHER C₄H₁₀O 250-500K

k(T) = - 7.0819597E-04 + 1.855898E-05T + 1.14117826E-07T²
k(250) = 0.01106 k(400) = 0.02497 k(500) = 0.0371
std error est = 1.8E-05 max error est = 1E-04

Note: Pressure dependence between 250-300K ignored.

250-500K

T(k) = 106.1 + 14272.722424k - 99605.2245926k²
T(0.01106) = 252 T(0.02497) = 400 T(0.0371) = 499
std error est = 0.9 max error est = 2.5

ETHYLENE C₂H₄ 200-450K

k(T) = 0.1690142 - 2.71392927E-03T + 1.71636899E-05T²
- 5.16435832E-08T³ + 7.74044499E-11T⁴ - 4.59993653E-14T⁵
k(200) = 8.75E-03 k(350) = 0.02743 k(450) = 0.04262
std error est = 7.0E-05 max error est = 1.2E-04

200-450K

T(k) = 108.663 + 12177.1554k - 168879.6154k² + 1672295.794854k³
T(8.75E-03) = 203 T(0.02743) = 350 T(0.04262) = 450
std error est = 1.3 max error est = 3.5

FLUORINE F₂ 90-800K

k(T) = 3.3854087E-04 + 8.27103562E-05T + 5.27622468E-08T²
- 7.51472474E-11T³
k(90) = 8.16E-03 k(400) = 0.03706 k(800) = 0.0618
std error est = 5.9E-05 max error est = 1E-04

Note: For T(k) calculations, use the iterative procedures discussed in Section 5 and the polynomial presented above.

HELIUM He 25-300K

k(T) = 1.028793E-02 + 8.51625139E-04T - 3.14258034E-06T²
+ 1.02188556E-08T³ - 1.3477236E-11T⁴
k(25) = 0.02977 k(200) = 0.1151 k(300) = 0.14969
std error est = 1.2E-04 max error est = 2E-04

HELIUM (continued)

300-500K

$$k(T) = -7.761491E-03 + \frac{8.66192033E-04}{T} - \frac{1.5559338E-06}{T^2}$$

$$+ \frac{1.40150565E-09}{T^3}$$

$$k(300) = 0.1499 \quad k(400) = 0.17946 \quad k(500) = 0.21154$$

$$\text{std error est} = 1.1E-04 \quad \text{max error est} = 2E-04$$

500-1500K

$$k(T) = -9.0656E-02 + \frac{9.37593087E-04}{T} - \frac{9.13347535E-07}{T^2}$$

$$+ \frac{5.55037072E-10}{T^3} - \frac{1.26457196E-13}{T^4}$$

$$k(500) = 0.21128 \quad k(1000) = 0.3622 \quad k(1500) = 0.4938$$

$$\text{std error est} = 8.9E-04 \quad \text{max error est} = 1.3E-03$$

1500-5000K

$$k(T) = 5.26198E-02 + \frac{3.31365073E-04}{T} - \frac{2.81816958E-08}{T^2}$$

$$+ \frac{2.1409764E-12}{T^3}$$

$$k(1500) = 0.4935 \quad k(3250) = 0.9054 \quad k(5000) = 1.2725$$

$$\text{std error est} = 2E-03 \quad \text{max error est} = 3E-03$$

100-5000K

$$T(k) = -99.57 + 2433.072575k + 1810.239628k^2 - 448.9582131k^3$$

$$T(0.1151) = 204 \quad T(0.4938) = 1489 \quad T(1.2725) = 5003$$

$$\underline{\text{std error est} = 6.5} \quad \underline{\text{max error est} = 15.0}$$
n-HEPTANE C_7H_{16} 250-1000K

$$k(T) = -4.606147E-02 + \frac{5.95652224E-04}{T} - \frac{2.98893153E-06}{T^2}$$

$$+ \frac{8.44612876E-09}{T^3} - \frac{1.2292738E-11}{T^4} + \frac{9.01270236E-15}{T^5}$$

$$- \frac{2.62961437E-18}{T^6}$$

$$k(250) = 0.0082 \quad k(500) = 0.0326 \quad k(1000) = 0.0971$$

$$\text{std error est} = 1.2E-04 \quad \text{max error est} = 4E-04$$

Note: Pressure dependence between 250-370K ignored.

250-1000K

$$T(k) = 156.21 + 12828.33732k - \frac{81042.0901}{k^2} + 390630.82849k^3$$

$$T(8.2E-03) = 256 \quad T(0.0326) = 502 \quad T(0.0971) = 995$$

$$\underline{\text{std error est} = 2.9} \quad \underline{\text{max error est} = 9.0}$$
n-HEXANE C_6H_{14} 250-1000K

$$k(T) = 1.287757E-03 - \frac{2.00499443E-05}{T} + \frac{2.37858831E-07}{T^2}$$

$$- \frac{1.60944555E-10}{T^3} + \frac{7.71027297E-14}{T^4}$$

$$k(250) = 8.9E-03 \quad k(600) = 0.0501 \quad k(1000) = 0.1353$$

$$\text{std error est} = 2.9E-04 \quad \text{max error est} = 6E-04$$
250-1000K

$$T(k) = 162.609 + 11501.7075k - \frac{63679.79437}{k^2} + 182669.90973k^3$$

$$T(8.9E-03) = 260 \quad T(0.0501) = 602 \quad T(0.1353) = 1006$$

$$\underline{\text{std error est} = 3.5} \quad \underline{\text{max error est} = 11.0}$$
HYDROGEN H_2 100-500K

$$k(T) = 2.009705E-02 + \frac{3.234622E-04}{T} + \frac{2.1637249E-06}{T^2}$$

$$- \frac{6.49151204E-09}{T^3} + \frac{5.52407932E-12}{T^4}$$

$$k(100) = 0.0681 \quad k(300) = 0.1813 \quad k(500) = 0.2566$$

HYDROGEN (continued)

std error est = 3.4E-04 max error est = 6E-04

$$\begin{aligned} & \text{500-1500K} \\ k(T) &= 0.1083105 + 2.21163789E-04T + 2.26380948E-07T^2 \\ &\quad - 1.74258636E-10T^3 + 4.6468625E-14T^4 \end{aligned}$$

$$\begin{aligned} k(500) &= 0.2566 & k(1000) &= 0.4281 & k(1500) &= 0.5965 \\ \text{std error est} &= 3.5E-04 & & & \text{max error est} &= 7E-04 \end{aligned}$$

$$\begin{aligned} & \text{1500-2000K} \\ k(T) &= -0.28107269 + 1.09703479E-03T - 5.27318283E-07T^2 \\ &\quad + 1.2403865E-10T^3 \end{aligned}$$

$$\begin{aligned} k(1500) &= 0.5966 & k(1750) &= 0.6886 & k(2000) &= 0.7960 \\ \text{std error est} &= 3.7E-04 & & & \text{max error est} &= 6E-04 \end{aligned}$$

$$\begin{aligned} & \text{100-500K} \\ T(k) &= -18.63 + 1990.8944k - 4723.849445k^2 + 19136.37907k^3 \\ T(0.0681) &= 101 & T(0.1813) &= 301 & T(0.2566) &= 505 \\ \text{std error est} &= 1.8 & & & \text{max error est} &= 5.5 \end{aligned}$$

$$\begin{aligned} & \text{500-1500K} \\ T(k) &= -228.573 + 2791.61736k + 187.56000746k^2 \\ T(0.2566) &= 500 & T(0.4281) &= 1001 & T(0.5965) &= 1503 \\ \text{std error est} &= 1.4 & & & \text{max error est} &= 5.0 \end{aligned}$$

$$\begin{aligned} & \text{1500-2000K} \\ T(k) &= -930.817 + 5242.1851374k - 1959.321732k^2 \\ T(0.5966) &= 1499 & T(0.6886) &= 1750 & T(0.796) &= 2001 \\ \text{std error est} &= 1.0 & & & \text{max error est} &= 3.0 \end{aligned}$$

HYDROGEN CHLORIDE HCl 200-700K

$$\begin{aligned} k(T) &= 1.2288265E-04 + 3.20474254E-05T + 1.02223086E-07T^2 \\ &\quad - 1.99696412E-10T^3 + 1.16463692E-13T^4 \\ k(200) &= 9.2E-03 & k(400) &= 0.0195 & k(700) &= 0.0321 \\ \text{std error est} &= 2.8E-05 & & & \text{max error est} &= 1E-04 \end{aligned}$$

$$\begin{aligned} & \text{200-700K} \\ T(k) &= 61.98 + 13391.474616k + 203362.8049798k^2 \\ T(9.2E-03) &= 202 & T(0.0195) &= 400 & T(0.0321) &= 701 \\ \text{std error est} &= 1.2 & & & \text{max error est} &= 2.5 \end{aligned}$$

HYDROGEN IODIDE HI 250-1000K

$$\begin{aligned} k(T) &= -4.35678828E-04 + 2.3083046E-05T - 3.77024198E-09T^2 \\ &\quad + 1.18389384E-12T^3 \\ k(250) &= 5.1E-03 & k(600) &= 0.0123 & k(1000) &= 0.0201 \\ \text{std error est} &= 2.7E-05 & & & \text{max error est} &= 1E-04 \end{aligned}$$

$$\begin{aligned} & \text{250-1000K} \\ T(k) &= 11.898 + 45338.55831k + 197725.8013557k^2 \\ T(5.1E-03) &= 248 & T(0.0123) &= 599 & T(0.0201) &= 1003 \\ \text{std error est} &= 1.4 & & & \text{max error est} &= 3.5 \end{aligned}$$

HYDROGEN SULFIDE H₂S 220-400K

k(T) = - 5.2404334E-03 + 6.7759251E-05T - 4.05425325E-09T²
k(220) = 0.0095 k(300) = 0.0147 k(400) = 0.0212
std error est = 2.9E-05 max error est = 1E-04

220-400K

T(k) = 77.82 + 14874.853457k + 14686.9999k²
T(9.5E-03) = 220 T(0.0147) = 300 T(0.0212) = 400
std error est = 0.5 max error est = 2.0

KRYPTON Kr 120-700K

k(T) = 4.6142E-05 + 3.48571058E-05T - 1.20386082E-08T²
k(120) = 4.06E-03 k(400) = 0.01206 k(700) = 0.01855
std error est = 1.7E-05 max error est = 1E-04

120-700K

T(k) = 21.254 + 22220.36563k + 761572.7864265k²
T(4.06E-03) = 124 T(0.01206) = 400 T(0.01855) = 696
std error est = 1.8 max error est = 4.5

METHANE CH₄ 100-1000K

k(T) = -1.3401499E-02 + 3.6630706E-04T - 1.82248608E-06T²
+ 5.93987998E-09T³ - 9.1405505E-12T⁴ + 6.7896889E-15T⁵
- 1.95048736E-18T⁶
k(100) = 0.0101 k(500) = 0.067 k(1000) = 0.169
std error est = 3E-04 max error est = 6E-04

100-1000K

T(k) = -19.358 + 11993.5848k - 98202.38989k² + 631750.65118k³
- 1542230.678766k⁴
T(0.0101) = 92 T(0.067) = 502 T(0.169) = 994
std error est = 2.8 max error est = 6.5

METHYL ALCOHOL CH₃OH 300-550K

k(T) = -2.0298675E-02 + 1.21910927E-04T - 2.23748473E-08T²
k(300) = 0.0143 k(425) = 0.0275 k(550) = 0.040
std error est = 3.8E-05 max error est = 1E-04

300-550K

T(k) = 173.252 + 8599.676374k + 20535.0012k²
T(0.0143) = 300 T(0.0275) = 425 T(0.040) = 550
std error est = 0.4 max error est = 1.5

METHYL CHLORIDE CH₃Cl 250-750K

k(T) = - 2.8950296E-03 + 2.42340563E-05T + 6.9670016E-08T²
k(250) = 7.5E-03 k(400) = 0.0179 k(750) = 0.0545
std error est = 1.1E-04 max error est = 2.5E-04

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50-500K

$k(T) = 2.201564E-03 + 2.27517163E-04T - 2.9729466E-07T^2$
 $+ 2.08844136E-10T^3$
 $k(50) = 0.0129 \quad k(250) = 0.0438 \quad k(500) = 0.0677$
 $\text{std error est} = 3.4E-05 \quad \text{max error est} = 1E-04$

500-1000K
 $k(T) = -0.0223377 + 2.83448846E-04T - 2.57636449E-07T^2$
 $+ 1.01142695E-10T^3$
 $k(500) = 0.0676 \quad k(750) = 0.088 \quad k(1000) = 0.1046$
 $\text{std error est} = 1.4E-04 \quad \text{max error est} = 2E-04$

1000-5000K
 $k(T) = 0.013526582 + 1.21904517E-04T - 4.05606888E-08T^2$
 $+ 1.14406524E-11T^3 - 1.65850704E-15T^4 + 9.29114306E-20T^5$
 $k(1000) = 0.1047 \quad k(2500) = 0.1878 \quad k(5000) = 0.2929$
 $\text{std error est} = 2.9E-04 \quad \text{max error est} = 4E-04$

50-500K
 $T(k) = 12.8374 + 2245.3161k + 73055.0207k^2$
 $T(0.0129) = 54 \quad T(0.0438) = 251 \quad T(0.0677) = 500$
 $\text{std error est} = 1.4 \quad \text{max error est} = 4$
500-1000K
 $T(k) = 1971.304 - 65338.30244k + 844869.0777k^2 - 2954030.585k^3$
 $T(0.0676) = 503 \quad T(0.088) = 751 \quad T(0.1046) = 1000$
 $\text{std error est} = 2.0 \quad \text{max error est} = 5.5$

1000-5000K
 $T(k) = -305.725 + 9215.50632k + 30228.47906k^2$
 $T(0.1047) = 991 \quad T(0.1878) = 2491 \quad T(0.2929) = 4987$
 $\text{std error est} = 9.0 \quad \text{max error est} = 14.5$

NITRIC OXIDE

NO

130-1000K

$k(T) = 2.695164E-03 + 3.8477785E-05T + 3.79042336E-07T^2$
 $- 1.3449086E-09T^3 + 2.15784789E-12T^4 - 1.64052333E-15T^5$
 $+ 4.79750187E-19T^6$
 $k(130) = 0.0117 \quad k(600) = 0.0462 \quad k(1000) = 0.0724$
 $\text{std error est} = 4.5E-05 \quad \text{max error est} = 1E-04$

130-1000K
 $T(k) = 20.91 + 7794.64895k + 140783.3849k^2 - 857527.26795k^3$
 $T(0.0117) = 130 \quad T(0.0462) = 597 \quad T(0.0724) = 998$
 $\text{std error est} = 2.1 \quad \text{max error est} = 4.5$

NITROGEN

N₂100-1500K

$k(T) = -1.5231785E-03 + 1.18879965E-04T - 1.2092845E-07T^2$
 $+ 1.15567802E-10T^3 - 6.36537349E-14T^4 + 1.47167023E-17T^5$
 $k(100) = 9.26E-03 \quad k(500) = 0.03861 \quad k(1500) = 0.0842$
 $\text{std error est} = 5.2E-05 \quad \text{max error est} = 2E-04$

NITROGEN (continued) 1500-3500K

$k(T) = 0.7282944 - 1.54313282E-03T + 1.3535933E-06T^2$
 $- 5.5158517E-10T^3 + 1.08449625E-13T^4 - 8.26807569E-18T^5$
 $k(1500) = 0.08382 \quad k(2500) = 0.14079 \quad k(3500) = 0.19131$
 $\text{std error est} = 3.2E-04 \quad \text{max error est} = 4E-04$

100-1500K

$T(k) = 38.19 + 5560.90414k + 186184.03159k^2 - 521677.344982k^3$
 $T(9.26E-03) = 105 \quad T(0.03861) = 500 \quad T(0.0842) = 1515$
 $\text{std error est} = 3.5 \quad \text{max error est} = 15.0$

1500-3500K

$T(k) = -15930.55 + 638350.15799k - 9332889.30298k^2 + 67699225.76k^3$
 $- 237257633.7266k^4 + 322622404.826k^5$
 $T(0.08382) = 1497 \quad T(0.14079) = 25 \quad T(0.19131) = 3497$
 $\text{std error est} = 5.5 \quad \text{max error est} = 12.5$

NITROGEN PEROXIDE NO₂ 440-640K

$k(T) = 8.90074818 - 8.02940254E-02T + 2.89756384E-04T^2$
 $- 5.2147063E-07T^3 + 4.6839284E-10T^4 - 1.6796286E-13T^5$
 $k(440) = 0.03309 \quad k(540) = 0.03752 \quad k(640) = 0.04479$
 $\text{std error est} = 4.1E-05 \quad \text{max error est} = 2E-04$

440-640K

$T(k) = -550.995 + 42497.74266k - 357393.73223k^2$
 $T(0.03309) = 464 \quad T(0.03752) = 540 \quad T(0.04479) = 635$
 $\text{std error est} = 7.5 \quad \text{max error est} = 15.0$

NITROUS OXIDE N₂O 190-1000K

$k(T) = 6.9918875E-03 - 7.16238986E-05T + 6.16971397E-07T^2$
 $- 1.13449444E-09T^3 + 9.64569615E-13T^4 - 3.11996398E-16T^5$
 $k(200) = 9.71E-03 \quad k(600) = 0.04182 \quad k(1000) = 0.07042$
 $\text{std error est} = 6.8E-05 \quad \text{max error est} = 1.2E-04$

190-1000K

$T(k) = 89.979 + 11746.9788k + 2979.32622k^2 + 193154.99479k^3$
 $T(9.71E-03) = 204 \quad T(0.04182) = 601 \quad T(0.07042) = 999$
 $\text{std error est} = 2.3 \quad \text{max error est} = 5.5$

n-NONANE C₉H₂₀ 250-1000K

$k(T) = -0.01073559242 + 7.71447107E-05T + 1.70209517E-10T^2$
 $k(250) = 8.56E-03 \quad k(600) = 0.03561 \quad k(1000) = 0.06658$
 $\text{std error est} = 3.0E-05 \quad \text{max error est} = 1E-04$

250-1000K

$T(k) = 139.123 + 12954.464853k - 366.184555k^2$
 $T(8.56E-03) = 250 \quad T(0.03561) = 600 \quad T(0.06658) = 1000$
 $\text{std error est} = 0.4 \quad \text{max error est} = 1.5$

n-OCTANE C₈H₁₈ 250-500K

k(T) = -4.0139194E-03 + 3.38796092E-05T + 8.19291819E-08T²
k(250) = 9.58E-03 k(400) = 0.02265 k(500) = 0.03341
std error est = 2.9E-05 max error est = 1E-04
Note: Pressure dependence between 250-390K ignored.

250-500K

T(k) = 121.451 + 14436.05859k - 93780.6879k²
T(9.58E-03) = 251 T(0.02265) = 400 T(0.03341) = 499
std error est = 0.6 max error est = 2.5

OXYGEN O₂ 100-1000K

k(T) = -7.6727798E-04 + 1.03560076E-04T - 4.62034365E-08T²
+ 1.51980292E-11T³
k(100) = 9.14E-03 k(600) = 0.04802 k(1000) = 0.07179
std error est = 9E-05 max error est = 2E-04
1000-1500K
k(T) = -0.18654526 + 7.05649428E-04T - 7.71025034E-07T²
+ 4.02143777E-10T³ - 7.84907953E-14T⁴
k(1000) = 0.07173 k(1250) = 0.0846 k(1500) = 0.097
std error est = 2E-05 max error est = 1E-04

100-1000K

T(k) = 11.465 + 9137.13572k + 65064.9850077k²
T(9.14E-03) = 100 T(0.04802) = 600 T(0.07179) = 1003
std error est = 1.2 max error est = 3.5

1000-1500K

T(k) = -212.8193 + 14703.836485k + 30477.8067k²
T(0.07173) = 999 T(0.0846) = 1249 T(0.097) = 1500
std error est = 1.0 max error est = 2.5

n-PENTANE C₅H₁₂ 250-500K

k(T) = -6.17042124E-03 + 5.06949328E-05T + 6.81013431E-08T²
k(250) = 0.01076 k(375) = 0.02242 k(500) = 0.0362
std error est = 3.2E-05 max error est = 1E-04
Note: Pressure dependence between 250-300K ignored.

250-500K

T(k) = 120.404 + 12797.2192k - 64302.207166k²
T(0.01076) = 251 T(0.02242) = 375 T(0.0362) = 499
std error est = 0.4 max error est = 2.5

PROPANE C₃H₈ 200-500K

k(T) = -1.07682209E-02 + 8.38590352E-05T + 4.22059864E-08T²
k(200) = 7.69E-03 k(350) = 0.02375 k(500) = 0.04171
std error est = 3.6E-05 max error est = 1E-04

PROPANE (continued) 200-500K

$$T(k) = 123.418 + 10224.285427k - 28865.4345095k^2$$

$$T(7.69E-03) = 200 \quad T(0.02375) = 350 \quad T(0.04171) = 500$$

$$\underline{\text{std error est}} = 0.4 \quad \underline{\text{max error est}} = 2.0$$

RADON Rn 200-1000K

$k(T) = -8.228225E-05 + 1.2546552E-05T + 7.9101118E-10T^2$
 $- 5.2693994E-12T^3 + 2.42034894E-15T^4$

$$k(200) = 2.52E-03 \quad k(600) = 6.91E-03 \quad k(1000) = 0.01041$$
 $\underline{\text{std error est}} = 1.5E-05 \quad \underline{\text{max error est}} = 1E-04$

200-1000K

$$T(k) = 37.13 + 61362.656052k + 2966201.713917k^2$$

$$T(2.52E-03) = 211 \quad T(6.91E-03) = 603 \quad T(0.01041) = 997$$
 $\underline{\text{std error est}} = 2.5 \quad \underline{\text{max error est}} = 11.5$

SULFUR DIOXIDE SO₂ 270-900K

$k(T) = -1.86270694E-02 + 3.19110134E-04T - 1.73644245E-06T^2$
 $+ 5.09847985E-09T^3 - 7.53585825E-12T^4 + 5.48078289E-15T^5$
 $- 1.56355469E-18T^6$

$$k(270) = 8.51E-03 \quad k(550) = 0.02285 \quad k(900) = 0.03998$$
 $\underline{\text{std error est}} = 1E-04 \quad \underline{\text{max error est}} = 3E-04$

270-900K

$$T(k) = 72.882 + 27366.02837k - 431142.085k^2 + 6765624.30409k^3$$

$$T(8.51E-03) = 279 \quad T(0.02285) \approx 554 \quad T(0.03998) = 910$$
 $\underline{\text{std error est}} = 4.5 \quad \underline{\text{max error est}} = 11.5$

TOLUENE C₇H₈ 250-600K

$k(T) = 5.33882E-02 - 4.90263636E-04T + 1.84066272E-06T^2$
 $- 2.5107707E-09T^3 + 1.28558132E-12T^4$

$$k(250) = 0.01165 \quad k(450) = 0.02943 \quad k(600) = 0.04615$$
 $\underline{\text{std error est}} = 4.9E-05 \quad \underline{\text{max error est}} = 1E-04$

250-600K

$$T(k) \approx 49.184 + 21881.4208k - 392934.468835k^2 + 3878149.983735k^3$$

$$T(0.01165) = 257 \quad T(0.02943) = 452 \quad T(0.04615) = 603$$
 $\underline{\text{std error est}} = 2.5 \quad \underline{\text{max error est}} = 8.0$

TRICHLOROFLUOROMETHANE CCl₃F 250-500K

(FREON-11)

$$k(T) \approx -4.57326E-03 + 4.23785103E-05T - 2.44200245E-09T^2$$

$$k(250) = 5.87E-03 \quad k(400) = 0.01199 \quad k(500) = 0.01601$$
 $\underline{\text{std error est}} = 2.5E-05 \quad \underline{\text{max error est}} = 1E-04$

Note: Pressure dependence between 250-300K ignored.

250-500K

$$T(k) = 108.8 + 23844.731142k + 37285.038633k^2$$

$$T(5.87E-03) = 250 \quad T(0.01199) = 400 \quad T(0.01601) = 500$$
 $\underline{\text{std error est}} = 0.7 \quad \underline{\text{max error est}} = 1.5$

TRICHLOROTRIFLUORO- $C_2Cl_3F_3$ 250-400K
 ETHANE (FREON-113)
 $k(T) = 6.2276996E-03 - 3.53066526E-05T + 1.33788515E-07T^2$
 $k(250) = 5.76E-03$ $k(350) = 0.01026$ $k(400) = 0.01351$
 $std\ error\ est = 2.1E-05$ $max\ error\ est = 1E-04$
 Note: Pressure dependence between 250-320K ignored.
250-400K
 $T(k) = -22.79 + 68493.0493k - 4352430.586665k^2 + 118681269.374k^3$
 $T(5.76E-03) = 250$ $T(0.01026) = 350$ $T(0.01351) = 401$
 $std\ error\ est = 0.6$ $max\ error\ est = 1.5$
 WATER (STEAM) H_2O 280-900K
 $k(T) = -2.65056964E-02 + 3.1147143E-04T - 9.84019456E-07T^2$
 $+ 1.92787663E-09T^3 - 1.68859732E-12T^4 + 5.48194497E-16T^5$
 $k(280) = 0.01644$ $k(500) = 0.0358$ $k(900) = 0.078$
 $std\ error\ est = 1.6E-04$ $max\ error\ est = 3E-04$
280-900K
 $T(k) = 28.726 + 17529.1632k - 157109.059k^2 + 971929.43672k^3$
 $T(0.01644) = 279$ $T(0.0358) = 500$ $T(0.078) = 901$
 $std\ error\ est = 1.6$ $max\ error\ est = 3.5$
 XENON Xe 200-750K
 $k(T) = 1.355426E-06 + 2.03984913E-05T - 5.53807454E-09T^2$
 $k(200) = 3.86E-03$ $k(500) = 8.82E-03$ $k(750) = 0.01219$
 $std\ error\ est = 3.9E-06$ $max\ error\ est = 1E-04$
200-750K
 $T(k) = 23.4897 + 40124.516223k + 1585115.24618k^2$
 $T(3.86E-03) = 202$ $T(8.82E-03) = 501$ $T(0.01219) = 748$
 $std\ error\ est = 1.0$ $max\ error\ est = 2.5$

APPENDIX C
TABLE C-I
SUMMARY OF CONTENTS

DYNAMIC VISCOSITY ($\times 10^{-6}$) OF
GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	APP C PAGE
Acetone	C ₃ H ₆ O	C-1
Acetylene	C ₂ H ₂	C-1
Air	-	C-1
Ammonia	NH ₃	C-1
Argon	Ar	C-2
Benzene	C ₆ H ₆	C-2
Bromine	Br ₂	C-2
Bromotrifluoromethane	CF ₃ Br	C-3
iso-Butane	i-C ₄ H ₁₀	C-3
n-Butane	n-C ₄ H ₁₀	C-3
Carbon Dioxide	CO ₂	C-3
Carbon Monoxide	CO	C-3
Carbon Tetrachloride	CCl ₄	C-4
Carbon Tetrafluoride	CF ₄	C-4
Chlorine	Cl ₂	C-4
Chlorodifluoromethane (FREON-22)	CHClF ₂	C-4
Chloroform	CHCl ₃	C-5
Chloropentafluoroethane	C ₂ ClF ₅	C-5
Chlorotrifluoromethane (FREON-13)	CClF ₃	C-5
Deuterium	D ₂	C-5
Dichlorodifluoromethane (FREON-12)	CCl ₂ F ₂	C-5
Dichlorofluoromethane (FREON-21)	CHCl ₂ F	C-6
Dichlorotetrafluoroethane (FREON-114)	C ₂ Cl ₂ F ₄	C-6
Ethane	C ₂ H ₆	C-6
Ethyl Alcohol	C ₂ H ₅ OH	C-6
Ethyl Ether	C ₄ H ₁₀ O	C-6
Ethylene	C ₂ H ₄	C-7
Fluorine	F ₂	C-7
Helium	He	C-7
n-Heptane	C ₇ H ₁₆	C-7
n-Hexane	C ₆ H ₁₄	C-8
Hydrogen	H ₂	C-8
Hydrogen Chloride	HCl	C-8
Hydrogen Iodide	HI	C-9

TABLE C-I
(CONT.)

NAME	FORMULA	APP C PAGE
Hydrogen Sulfide	H ₂ S	C-9
Iodine	I ₂	C-9
Krypton	Kr	C-9
Methane	CH ₄	C-10
Methyl Alcohol	CH ₃ OH	C-10
Methyl Chloride	CH ₃ Cl	C-10
Neon	Ne	C-10
Nitric Oxide	NO	C-11
Nitrogen	N ₂	C-11
Nitrogen Peroxide	NO ₂	C-11
Nitrous Oxide	N ₂ O	C-11
Octafluorocyclobutane	C ₄ F ₈	C-12
n-Octane	C ₈ H ₁₈	C-12
Oxygen	O ₂	C-12
n-Pentane	C ₅ H ₁₂	C-12
Propane	C ₃ H ₈	C-12
Propylene	C ₃ H ₆	C-13
Sulfur Dioxide	SO ₂	C-13
Toluene	C ₇ H ₈	C-13
Trichlorofluoromethane (FREON-11)	CCl ₃ F	C-13
Trichlorotrifluoroethane (FREON-113)	C ₂ Cl ₃ F ₃	C-13
Trifluoromethane	CHF ₃	C-14
Water	H ₂ O ³	C-14
Xenon	Xe	C-14

APPENDIX C
FORMAT EXAMPLE

The equations presented are for gaseous Acetylene

The polynomial equation to calculate the dynamic viscosity (μ) in N s/m² as a function of temperature (Kelvin)

ACETYLENE	Formula	Valid temperature range
	C_2H_2	<u>270-600K</u>
	$\mu(T) = -0.4486325 + 3.92559E-02T - 1.1077158E-05T^2$	
	$\mu(270) = 9.34$	$\mu(400) = 13.48$
	std error est = 4.04E-03	$\mu(600) = 19.12$
		max error est = 0.01
		<u>270-600K</u>
	$T(\mu) = 31.82 + 21.5671447\mu + 0.4252123\mu^2$	
	$T(9.34) = 270$	$T(13.48) = 400$
	std error est = 0.3	$T(19.12) = 600$
	standard (or average) error estimate is ±0.3 degrees Kelvin	max_error_est = 1.5
		Using the polynomial presented, the calculated temperature for a given $\mu = 19.12E-06N s/m^2$ is 600K.

***Note: All of the values for dynamic viscosity (μ) MUST be multiplied by 1E-06.

FIGURE C-1

APPENDIX C

DYNAMIC VISCOSITY (x 1E-06) OF
GASEOUS ELEMENTS AND COMPOUNDS

ACETONE	C_3H_6O	<u>250-650K</u>
$\mu(T) = 3.996401 + 1.51018819E-03T + 4.44247E-05T^2 - 2.47973E-08T^3$		
$\mu(250) = 6.76$	$\mu(400) = 10.12$	$\mu(650) = 16.94$
std error est = 1.906E-02		max error est = 0.04
	<u>250-650K</u>	
$T(\mu) = -191.27 + 84.748208\mu - 3.388215\mu^2 + 7.7871645E-02\mu^3$		
$T(6.76) = 251$	$T(10.12) = 400$	$T(16.94) = 651$
std error est = 0.9		max error est = 2
ACETYLENE	C_2H_2	<u>270-600K</u>
$\mu(T) = -0.4486325 + 3.92559E-02T - 1.1077158E-05T^2$		
$\mu(270) = 9.34$	$\mu(400) = 13.48$	$\mu(600) = 19.12$
std error est = 4.04E-03		max error est = 0.01
	<u>270-600K</u>	
$T(\mu) = 31.82 + 21.5671447\mu + .42521234\mu^2$		
$T(9.34) = 270$	$T(13.48) = 400$	$T(19.12) = 600$
std error est = 0.3		max error est = 1.5
AIR		<u>80-600K</u>
$\mu(T) = -0.98601 + 0.09080125T - 1.17635575E-04T^2 + 1.2349703E-07T^3$		
$- 5.7971299E-11T^4$		
$\mu(80) = 5.59$	$\mu(350) = 20.81$	$\mu(600) = 30.31$
std error est = 1.47E-02		max error est = 0.07
	<u>600-2000K</u>	
$\mu(T) = 4.8856745 + 5.43232E-02T - 2.4261775E-05T^2 + 7.9306E-09T^3$		
$- 1.10398E-12T^4$		
$\mu(600) = 30.32$	$\mu(1200) = 46.55$	$\mu(2000) = 62.27$
std error est = 1.98E-02		max error est = 0.05
	<u>80-600K</u>	
$T(\mu) = 23.211 + 8.59256\mu + 0.342764\mu^2$		
$T(5.59) = 82$	$T(20.81) = 350$	$T(30.31) = 600$
std error est = 0.7		max error est = 1.5
	<u>600-2000K</u>	
$T() = 92.81 + 3.601092\mu + 0.43380968\mu^2$		
$T(30.32) = 601$	$T(46.55) = 1200$	$T(62.27) = 1999$
std error est = 1.0		max error est = 2.5
AMMONIA	NH_3	<u>200-1000K</u>
$\mu(T) = 0.3639 + 2.999278E-02T + 1.25282E-05T^2 - 7.033645E-09T^3$		
$\mu(200) = 6.81$	$\mu(600) = 21.35$	$\mu(1000) = 35.85$
std error est = 3.57E-02		max error est = 0.08

AMMONIA (continued) 200-1000K
 $T(\mu) = 20.22 + 27.09159\mu + 2.94502348E-03\mu^2$
 $T(6.81) = 205 \quad T(21.35) = 600 \quad T(35.85) = 995$
 $\underline{\text{std error est}} = 2.2 \quad \underline{\text{max error est}} = 5.0$
 ARGON Ar 60-540K
 $\mu(T) = 1.22573 + 5.9456964E-02T + 1.897011E-04T^2 - 8.171242E-07T^3$
 $+ 1.2939183E-09T^4 - 7.5027442E-13T^5$
 $\mu(60) = 5.32 \quad \mu(350) = 25.72 \quad \mu(540) = 35.55$
 $\text{std error est} = 1.95E-02 \quad \text{max error est} = 0.03$
540-2200K
 $\mu(T) = 4.03764 + 7.3665688E-02T - 3.3867E-05T^2 + 1.127158E-08T^3$
 $- 1.585569E-12T^4$
 $\mu(540) = 35.58 \quad \mu(1250) = 61.35 \quad \mu(2200) = 85.06$
 $\text{std error est} = 0.03 \quad \text{max error est} = 0.05$
60-540K
 $T(\mu) = 12.722 + 9.0267675\mu + 0.161221378\mu^2$
 $T(5.32) = 65 \quad T(25.72) = 351 \quad T(35.55) = 537$
 $\text{std error est} = 1.7 \quad \text{max error est} = 5.0$
540-2200K
 $\mu(T) = 108.244 + 3.305827\mu + 0.24958985\mu^2$
 $T(35.58) = 542 \quad T(61.35) = 1250 \quad T(85.06) = 2195$
 $\underline{\text{std error est}} = 1.1 \quad \underline{\text{max error est}} = 5.0$
 BENZENE C₆H₆ 270-650K
 $\mu(T) = 0.39324 + 2.24768E-02T + 8.090553E-06T^2 - 7.8349307E-09T^3$
 $\mu(270) = 6.90 \quad \mu(400) = 10.18 \quad \mu(650) = 16.27$
 $\text{std error est} = 0.02 \quad \text{max error est} = 0.04$
270-650K
 $T(\mu) = 12.343 + 36.249\mu + 0.177428\mu^2$
 $T(6.90) = 272 \quad T(10.18) = 400 \quad T(16.27) = 649$
 $\underline{\text{std error est}} = 0.9 \quad \underline{\text{max error est}} = 2.0$
 BORON TRIFLUORIDE BF₃ 190-700K
 $\mu(T) = 1.401165 + 5.644982E-02T - 1.4088857E-05T^2$
 $\mu(190) = 11.62 \quad \mu(400) = 21.73 \quad \mu(700) = 34.01$
 $\text{std error est} = 1.9E-02 \quad \text{max error est} = 0.03$
190-700K
 $T(\mu) = -38.33 + 19.737077\mu - 0.0468724\mu^2 + 3.08592457E-03\mu^3$
 $T(11.62) = 190 \quad T(21.73) = 400 \quad T(34.01) = 700$
 $\underline{\text{std error est}} = 0.5 \quad \underline{\text{max error est}} = 1.5$
 BROMINE Br₂ 280-800K
 $\mu(T) = 0.8027126 + 4.9413942E-02T - 1.70534854E-06T^2$
 $\mu(280) = 14.50 \quad \mu(500) = 25.08 \quad \mu(800) = 39.24$
 $\text{std error est} = 4.35E-02 \quad \text{max error est} = 0.21$

BROMINE (continued) 280-800K
 $\mu(T) = -51.3 + 24.52145\mu - 0.153459363\mu^2 + 2.0985285E-03\mu^3$
 $T(14.50) = 278 \quad T(25.08) = 500 \quad T(39.24) = 801$
~~std error est = 0.7~~ ~~max error est = 1.5~~

BROMOTRIFLUOROMETHANE CF_3Br 230-500K
 $\mu(T) = -1.62177 + 0.0694797T - 4.550649E-05T^2 + 2.0833526E-08T^3$
 $\mu(230) = 12.20 \quad \mu(350) = 18.01 \quad \mu(500) = 24.35$
~~std error est = 0.02~~ ~~max error est = 0.09~~

230-500K
 $T(\mu) = 33.415 + 13.0473238\mu + 0.25127636\mu^2$
 $T(12.20) = 230 \quad T(18.01) = 350 \quad T(24.35) = 500$
~~std error est = 0.4~~ ~~max error est = 1.5~~

iso-BUTANE $i-C_4H_{10}$ 270-520K
 $\mu(T) = -0.102505 + 2.6972076E-02T - 4.2918193E-06T^2$
 $\mu(270) = 6.87 \quad \mu(400) = 10.00 \quad \mu(520) = 12.76$
~~std error est = 6.5E-03~~ ~~max error est = 0.02~~

270-520K
 $T(\mu) = 7.628 + 35.967103\mu + 0.3272017\mu^2$
 $T(6.87) = 270 \quad T(10.00) = 400 \quad T(12.76) = 520$
~~std error est = 0.3~~ ~~max error est = 1.5~~

n-BUTANE $n-C_4H_{10}$ 270-520K
 $\mu(T) = -0.01099487 + 2.634504E-02T - 3.54700854E-06T^2$
 $\mu(270) = 6.84 \quad \mu(400) = 9.96 \quad \mu(520) = 12.73$
~~std error est = 5.9E-03~~ ~~max error est = 0.02~~

270-520K
 $T(\mu) = 3.12 + 37.1408242\mu + 0.271992359\mu^2$
 $T(6.84) = 270 \quad T(9.96) = 400 \quad T(12.73) = 520$
~~std error est = 0.3~~ ~~max error est = 1.5~~

CARBON DIOXIDE CO_2 170-2000K
 $\mu(T) = -0.8095191 + 6.0395329E-02T - 2.824853E-05T^2 + 9.843776E-09T^3$
 $- 1.47315277E-12T^4$
 $\mu(170) = 8.69 \quad \mu(1100) = 42.39 \quad \mu(2000) = 62.17$
~~std error est = 3E-02~~ ~~max error est = 0.1~~

170-2000K
 $T(\mu) = 25.166 + 15.2582\mu + 0.1780093719\mu^2 + 1.4129E-03\mu^3$
 $T(8.69) = 172 \quad T(42.39) = 1099 \quad T(62.17) = 2001$
~~std error est = 1.3~~ ~~max error est = 5.0~~

CARBON MONOXIDE CO 80-1500K
 $\mu(T) = -0.524575 + 7.9606E-02T - 7.82295E-05T^2 + 6.2821488E-08T^3$
 $- 2.83747E-11T^4 + 5.317831E-15T^5$
 $\mu(80) = 5.37 \quad \mu(800) = 35.38 \quad \mu(1500) = 51.63$

CARBON MONOXIDE (continued)

std error est = 2.62E-02 max error est = 0.03

$$T(\mu) = 21.08 + 10.0217\mu + \frac{80-1500K}{0.289517\mu^2} + 1.4002864E-03\mu^3$$

T(5.37) = 83 T(35.38) = 800 T(51.63) = 1503

std error est = 1.3 max error est = 3.5

CARBON TETRACHLORIDE CC₄ 280-800K

$$\mu(T) = -1.5110416 + 4.3798388E-02T - 2.02626E-05T^2 + 6.144E-09T^3$$

$\mu(280) = 9.30 \quad \mu(550) = 17.47 \quad \mu(800) = 23.71$

std error est = 2.2E-02 max error est = 0.04

$$T(\mu) = 53.258 + 19.890474\mu + \frac{280-800K}{0.489386918\mu^2}$$

T(9.30) = 281 T(17.47) = 550 T(23.71) = 800

std error est = 0.9 max error est = 2.5

CARBON TETRAFLUORIDE CF₄ 230-500K

$$\mu(T) = -1.235676 + 7.815327E-02T - 6.115548E-05T^2 + 2.95168E-08T^3$$

$\mu(230) = 13.86 \quad \mu(400) = 22.13 \quad \mu(500) = 26.24$

std error est = 2.7E-03 max error est = 0.01

$$T(\mu) = 37.74 + 9.70199\mu + \frac{230-500K}{0.30144808\mu^2}$$

T(13.86) = 230 T(22.13) = 400 T(26.24) = 500

std error est = 0.1 max error est = 1.0

CHLORINE Cl₂ 270-800K

$$\mu(T) = -1.81447 + 5.814046E-02T - 2.299287E-05T^2 + 5.015775E-09T^3$$

$\mu(270) = 12.31 \quad \mu(550) = 24.04 \quad \mu(800) = 32.55$

std error est = 0.08 max error est = 0.15

$$T(\mu) = 56.456 + 14.237878\mu + \frac{270-800K}{0.262332581\mu^2}$$

T(12.31) = 271 T(24.04) = 550 T(32.55) = 798

std error est = 2.5 max error est = 5.0

CHLORODIFLUOROMETHANE CHClF₂ 250-500K

(FREON-22)

$$\mu(T) = -0.7369597 + 4.9394676E-02T - 1.2112332E-05T^2$$

$\mu(250) = 10.85 \quad \mu(400) = 17.08 \quad \mu(500) = 20.93$

std error est = 0.02 max error est = 0.03

$$T(\mu) = 23.086 + 18.911\mu + \frac{250-500K}{0.18471282\mu^2}$$

T(10.85) = 250 T(17.08) = 400 T(20.93) = 500

std error est = 0.3 max error est = 2.0

CHLOROFORM **CHCl₃** **250-650K**

$\mu(T) = -0.389489 + 3.6808E-02T - 2.72048E-06T^2 - 3.194456E-09T^3$
 $\mu(250) = 8.59 \quad \mu(450) = 15.33 \quad \mu(650) = 21.51$
 std error est = 0.022 max error est = 0.09

$$T(\mu) = 23.48 + 24.644568\mu + \frac{250-650K}{0.207098\mu^2}$$

T(8.59) = 250 T(15.33) = 450 T(21.51) = 649
 std error est = 0.8 max error est = 3.5

CHLOROPENTAFLUOROETHANE C₂C₁F₅ 250-500K

$\mu(T) = 0.357912 + 4.440886E-02T - 1.014652E-05T^2$
 $\mu(250) = 10.83 \quad \mu(400) = 16.50 \quad \mu(500) = 20.03$
 std error est = 3.5E-03 max error est = 0.01

$T(\mu) = 0.2646 + 20.875165\mu + 0.203445135\mu^2$
 $T(10.83) = 250 \quad T(16.50) = 400 \quad T(20.03) = 500$
 std error est = 0.2 max error est = 1.0

CHLOROTRIFLUOROMETHANE CC₁F₃ 230-500K

(FREON-13) $\mu(T) = 4.018574 + 2.3020865E-02T + 5.190552E-05T^2 - 4.09445E-08T^3$
 $\mu(230) = 11.56 \quad \mu(400) = 18.91 \quad \mu(500) = 23.39$
 std error est = 4.4E-03 max error est = 0.01

$$\begin{aligned} T(\mu) &= -53.645 + 25.566055\mu - 8.24565722E-02\mu^2 \\ T(11.56) &= 231 \quad T(18.91) = 400 \quad T(23.39) = 499 \\ \text{std error est} &= 0.5 \quad \text{max error est} = 2.5 \end{aligned}$$

DEUTERIUM D₂ 15-500K

$$\mu(T) = -0.0374066 + 0.07422285T - 1.98491852E-04T^2 + 4.0366E-07T^3 - 3.18855544E-10T^4$$

$\mu(15) = 1.03$ $\mu(300) = 12.68$ $\mu(500) = 17.98$
std error est = 4.5E-02 max error est = 0.09

$$T(\mu) = -0.449 + 13.1729602\mu + \frac{15-500K}{0.8102567096\mu^2}$$

$$T(1.03) = 14 \quad T(12.68) = 297 \quad T(17.98) = 498$$

DIGITAL PROFILE VEROMETRUM 261 E 250 5000

$$\begin{aligned} & \text{CHLORODIFLUOROMETHANE } \text{CCl}_2\text{F}_2 \text{ } 250-500 \\ & (\text{FREON-12}) \\ & \mu(T) = -0.904423 + 5.03878E-02T - 1.7884615E-05T^2 \\ & \mu(250) = 10.57 \quad \mu(400) = 16.39 \quad \mu(500) = 19.82 \\ & \text{at } 25^\circ\text{C} = 5.35 \text{ E-02} \quad \text{at } 50^\circ\text{C} = 0.01 \end{aligned}$$

DICHLORODIFLUOROMETHANE (continued) 250-500K

$T(\mu) = 38.998 + 16.2507676\mu + 0.3528873\mu^2$
 $T(10.57) = 250 \quad T(16.39) = 400 \quad T(19.82) = 500$
std error est = 0.2 max error est = 1.5

DICHLOROFLUOROMETHANE CHCl_2F 280-500K

(FREON-21)
 $\mu(T) = 0.033118573 + 4.03724167E-02T - 5.7792208E-06T^2$
 $\mu(280) = 10.88 \quad \mu(400) = 15.26 \quad \mu(500) = 18.77$
std error est = 5.8E-03 max error est = 0.01

280-500K
 $T(\mu) = 2.23 + 24.1579854\mu + 0.1253726\mu^2$

$T(10.88) = 280 \quad T(15.26) = 400 \quad T(18.77) = 500$
std error est = 0.2 max error est = 1.5

DICHLOROTETRAFLUOROETHANE $\text{C}_2\text{Cl}_2\text{F}_4$ 230-500K

(FREON-114)
 $\mu(T) = 4.649332 + 9.784407E-03T + 5.818667E-05T^2 - 4.542242E-08T^3$
 $\mu(230) = 9.43 \quad \mu(400) = 14.97 \quad \mu(500) = 18.41$
std error est = 6.2E-03 max error est = 0.01

230-500K
 $T(\mu) = -87.64 + 35.9444125\mu - 0.2222265\mu^2$

$T(9.43) = 232 \quad T(14.97) = 401 \quad T(18.41) = 499$
std error est = 0.7 max error est = 2.5

ETHANE C_2H_6 190-1000K

$\mu(T) = -0.5107728 + 3.76582E-02T - 1.59412113E-05T^2 + 3.906E-09T^3$
 $\mu(190) = 6.10 \quad \mu(600) = 17.19 \quad \mu(1000) = 25.11$
std error est = 3.3E-02 max error est = 0.03

190-1000K
 $T(\mu) = 43.829 + 20.323073\mu + 0.7026353\mu^2$

$T(6.10) = 194 \quad T(17.19) = 601 \quad T(25.11) = 997$
std error est = 2.2 max error est = 4.5

ETHYL ALCOHOL $\text{C}_2\text{H}_5\text{OH}$ 270-600K

$\mu(T) = -0.0633595 + 3.2071347E-02T - 6.25079576E-06T^2$
 $\mu(270) = 8.14 \quad \mu(400) = 11.77 \quad \mu(600) = 16.93$
std error est = 3.9E-03 max error est = 0.01

270-600K
 $T(\mu) = 10.415 + 29.22028895\mu + 0.330513733\mu^2$

$T(8.14) = 270 \quad T(11.77) = 400 \quad T(16.93) = 600$
std error est = 0.2 max error est = 1.5

ETHYL ETHER $\text{C}_4\text{H}_{10}\text{O}$ 250-650K

$\mu(T) = -0.82017 + 2.98341946E-02T - 4.938627E-06T^2 - 2.82999E-09T^3$
 $\mu(250) = 6.29 \quad \mu(450) = 11.35 \quad \mu(650) = 15.71$

ETHYL ETHER (continued)

std error est = 0.02 max error est = 0.03
 $T(\mu) = 51.2 + 27.634314\mu + 0.6622779\mu^2$
 $T(6.29) = 251 \quad T(11.35) = 450 \quad T(15.71) = 649$
 std error est = 0.9 max error est = 3.5
 - - - - -

ETHYLENE C₂H₄ 190-1500K

$\mu(T) = -0.3919492 + 0.040557T - 1.6439973E-05T^2 + 3.7310454E-09T^3$
 $\mu(190) = 6.75 \quad \mu(800) = 23.44 \quad \mu(1500) = 36.05$
 std error est = 2.6E-02 max error est = 0.05
 $T(\mu) = 23.3 + 22.4670445\mu + 0.34307964\mu^2 + 4.8478305E-03\mu^3$
 $T(6.75) = 192 \quad T(23.44) = 801 \quad T(36.05) = 1506$
 std error est = 1.1 max error est = 6.5

FLUORINE F₂ 90-500K

$\mu(T) = -1.3474535 + 0.1088684T - 1.032287E-04T^2 + 6.02076E-08T^3$
 $\mu(90) = 7.66 \quad \mu(350) = 26.69 \quad \mu(500) = 34.81$
 std error est = 3E-02 max error est = 0.1
 $T(\mu) = 23.06 + 7.555066\mu + 0.176432568\mu^2$
 $T(7.66) = 91 \quad T(26.69) = 350 \quad T(34.81) = 500$
 std error est = 0.7 max error est = 2.5

HELIUM He 1-500K

$\mu(T) = 0.39414 + 0.17213335T - 1.38733E-03T^2 + 8.020045E-06T^3$
 $- 2.4278655E-08T^4 + 3.641644E-11T^5 - 2.14117E-14T^6$
 $\mu(1) = 0.56 \quad \mu(250) = 17.53 \quad \mu(500) = 28.17$
 std error est = 9.2E-02 max error est = 0.19

$\mu(T) = 7.442412 + 4.6649873E-02T - 1.0385665E-05T^2 + 1.35269E-09T^3$
 $\mu(500) = 28.34 \quad \mu(1500) = 58.61 \quad \mu(2500) = 80.29$
 std error est = 4E-02 max error est = 0.09

$T(\mu) = -2.78 + 4.7805365\mu + 0.702059\mu^2 - 8.7384854E-03\mu^3$
 $T(.56) = 0 \quad T(17.53) = 250 \quad T(28.17) = 494$
 std error est = 2.2 max error est = 7.0

$T(\mu) = -15.4944 + 11.26614\mu + 0.249906096\mu^2$
 $T(28.34) = 505 \quad T(58.61) = 1503 \quad T(80.29) = 2500$
 std error est = 1.9 max error est = 5.5

n-HEPTANE C₇H₁₆ 270-580K

n-HEPTANE (continued) 270-580K
 $\mu(T) = 1.540097 + 1.095157E-02T + 1.800664E-05T^2 - 1.36379E-08T^3$
 $\mu(270) = 5.54 \quad \mu(400) = 7.93 \quad \mu(580) = 11.29$
 $\text{std error est} = 3.1E-03 \quad \text{max error est} = 0.01$
270-580K
 $T(\mu) = -31.9 + 55.191463\mu - 9.495688E-02\mu^2$
 $T(5.54) = 271 \quad T(7.93) = 400 \quad T(11.29) = 579$
 ~~$\text{std error est} = 0.6$~~ ~~$\text{max error est} = 1.5$~~
n-HEXANE C₆H₁₄ 270-900K

$\mu(T) = 1.545412 + 1.150809E-02T + 2.722165E-05T^2 - 3.269E-08T^3$
 $+ 1.245459E-11T^4$
 $\mu(270) = 6.06 \quad \mu(600) = 12.80 \quad \mu(900) = 18.29$
 $\text{std error est} = 4.6E-03 \quad \text{max error est} = 0.01$
270-900K
 $T(\mu) = -35.27 + 53.9008\mu - 0.760933\mu^2 + 3.349925E-02\mu^3$
 $T(6.06) = 271 \quad T(12.80) = 600 \quad T(18.29) = 901$
 ~~$\text{std error est} = 0.5$~~ ~~$\text{max error est} = 2.0$~~
HYDROGEN H₂ 10-500K

$\mu(T) = -0.135666 + 6.84115878E-02T - 3.928747E-04T^2 + 1.8996E-06T^3$
 $- 5.23104E-09T^4 + 7.4490972E-12T^5 - 4.250937E-15T^6$
 $\mu(10) = 0.51 \quad \mu(250) = 7.90 \quad \mu(500) = 12.72$
 $\text{std error est} = 9.6E-03 \quad \text{max error est} = 0.03$
500-2000K
 $T(\mu) = 2.72941 + 2.3224377E-02T - 7.6287854E-06T^2 + 2.92585E-09T^3$
 $- 5.2889938E-13T^4$
 $\mu(500) = 12.77 \quad \mu(1250) = 24.26 \quad \mu(2000) = 33.61$
 $\text{std error est} = 3.3E-02 \quad \text{max error est} = 0.05$
10-500K
 $T(\mu) = -7.126 + 19.551451\mu + 1.6191086\mu^2$
 $T(0.51) = 3 \quad T(7.90) = 248 \quad T(12.72) = 503$
 $\text{std error est} = 2.9 \quad \text{max error est} = 7.0$
500-2000K
 $T(\mu) = -116.25 + 39.399135\mu + 0.69646657\mu^2$
 $T(12.77) = 500 \quad T(24.26) = 1249 \quad T(33.61) = 1995$
 ~~$\text{std error est} = 2.5$~~ ~~$\text{max error est} = 6.0$~~
HYDROGEN CHLORIDE HCl 250-650K

$(T) = -10.37895 + 0.146304667T - 3.3750673E-04T^2 + 5.204805E-07T^3$
 $- 3.066023E-10T^4$
 $(250) = 12.04 \quad (450) = 21.97 \quad (650) = 30.33$
 $\text{std error est} = 0.143 \quad \text{max error est} = 0.25$

HYDROGEN CHLORIDE (continued) 250-650K

$$T(\mu) = 54.8 + 14.1533\mu + 0.17335227\mu^2$$

$$T(12.04) = 250 \quad T(21.97) = 449 \quad T(30.33) = 644$$

std error est = 3.9 max error est = 7.5

HYDROGEN IODIDE HI 250-650K

$$\mu(T) = -0.8210072 + 6.96502E-02T - 1.1987247E-05T^2$$

$$\mu(250) = 15.84 \quad \mu(400) = 25.12 \quad \mu(650) = 39.39$$

std error est = 2.6E-02 max error est = 0.09

$$T(\mu) = 18.0 + 13.73048\mu + 5.8615567E-02\mu^2$$

$$T(15.84) = 250 \quad T(25.12) = 400 \quad T(39.39) = 650$$

std error est = 0.6 max error est = 2.0

HYDROGEN SULFIDE H₂S 270-500K

$$\mu(T) = -1.880078 + 5.29022575E-02T - 1.49125874E-05T^2$$

$$\mu(270) = 11.32 \quad \mu(400) = 16.89 \quad \mu(500) = 20.84$$

std error est = 1.6E-02 max error est = 0.03

$$T(\mu) = 46.59 + 17.386465\mu + 0.2091804\mu^2$$

$$T(11.32) = 270 \quad T(16.89) = 400 \quad T(20.84) = 500$$

std error est = 0.5 max error est = 1.5

IODINE I₂ 370-700K

$$\mu(T) = -9.77787 + 0.12652959T - 2.34192527E-04T^2 + 2.94743E-07T^3$$

$$- 1.409635E-10T^4$$

$$\mu(370) = 17.26 \quad \mu(550) = 25.11 \quad \mu(700) = 31.29$$

std error est = 4E-02 max error est = 0.04

$$T(\mu) = 11.76 + 19.2390557\mu + 8.7220577E-02\mu^2$$

$$T(17.26) = 370 \quad T(25.11) = 550 \quad T(31.29) = 699$$

std error est = 0.9 max error est = 2.5

KRYPTON Kr 100-1500K

$$\mu(T) = -0.465233 + 9.9000315E-02T - 4.278998E-05T^2 + 1.9612E-09T^3$$

$$+ 1.0362237E-11T^4 - 3.592904E-15T^5$$

$$\mu(100) = 9.01 \quad \mu(800) = 55.42 \quad \mu(1500) = 83.55$$

std error est = 5.5E-02 max error est = 0.3

$$T(\mu) = 15.03 + 9.1084\mu + 6.7458509E-02\mu^2 + 4.33414E-04\mu^3$$

$$T(9.01) = 103 \quad T(55.42) = 801 \quad T(83.55) = 1500$$

std error est = 1.3 max error est = 6.5

METHANE CH₄ 70-1000K

$$\mu(T) = 0.2968267 + 3.711201E-02T + 1.218298E-05T^2 - 7.02426E-08T^3 \\ + 7.543269E-11T^4 - 2.7237166E-14T^5$$

$$\mu(70) = 2.93 \quad \mu(550) = 18.24 \quad \mu(1000) = 27.54 \\ \text{std error est} = 3E-02 \quad \text{max error est} = 0.09$$

$$70-1000K \quad T(\mu) = 2.184 + 23.32102\mu + 0.179160065\mu^2 + 1.0455235E-02\mu^3 \\ T(2.93) = 72 \quad T(18.24) = 551 \quad T(27.54) = 999$$

$$\text{std error est} = 1.4 \quad \text{max error est} = 3.5$$

METHYL ALCOHOL CH₃OH 250-650K

$$\mu(T) = 1.1979 + 0.0245028T + 1.8616274E-05T^2 - 1.3067482E-08T^3 \\ \mu(250) = 8.28 \quad \mu(400) = 13.14 \quad \mu(650) = 21.40 \\ \text{std error est} = 3.2E-02 \quad \text{max error est} = 0.04$$

$$250-650K \quad T(\mu) = -4.983 + 31.162925\mu - 2.8760994E-02\mu^2 \\ T(8.28) = 251 \quad T(13.14) = 400 \quad T(21.40) = 649 \\ \text{std error est} = 1.1 \quad \text{max error est} = 2.5$$

METHYL CHLORIDE CH₃Cl 250-660K

$$\mu(T) = 0.282322 + 0.0364907T - 2.48976E-06T^2 \\ \mu(250) = 9.25 \quad \mu(400) = 14.48 \quad \mu(660) = 23.28 \\ \text{std error est} = 2.4E-02 \quad \text{max error est} = 0.04$$

$$250-660K \quad T(\mu) = -6.86 + 27.202172\mu + 6.180147E-02\mu^2 \\ T(9.25) = 250 \quad T(14.48) = 400 \quad T(23.28) = 660 \\ \text{std error est} = 0.7 \quad \text{max error est} = 2.0$$

NEON Ne 20-450K

$$\mu(T) = -0.261473 + 0.2007328T - 7.54726E-04T^2 + 2.5795522E-06T^3 \\ - 4.7146844E-09T^4 + 3.3937307E-12T^5 \\ \mu(20) = 3.47 \quad \mu(250) = 27.95 \quad \mu(450) = 41.59 \\ \text{std error est} = 4E-02 \quad \text{max error est} = 0.09$$

$$450-1200K \quad \mu(T) = 9.5675148 + 8.4038686E-02T - 3.2087447E-05T^2 + 7.366716E-09T^3 \\ \mu(450) = 41.56 \quad \mu(850) = 62.34 \quad \mu(1200) = 76.94 \\ \text{std error est} = 2.9E-02 \quad \text{max error est} = 0.06$$

$$20-450K \quad T(\mu) = 0.08 + 4.9693056\mu + 0.141318424\mu^2 \\ T(3.47) = 19 \quad T(27.95) = 249 \quad T(41.59) = 451 \\ \text{std error est} = 0.5 \quad \text{max error est} = 2.5$$

NEON (continued) 450-1200K
 $T(\mu) = -1.85 + 5.337484\mu + 0.1336294\mu^2$
 $T(41.56) = 451 \quad T(62.34) = 850 \quad T(76.94) = 1200$
~~- std error est = 0.6~~ ~~max error est = 2.0~~
 NITRIC OXIDE NO 110-1500K
 $\mu(T) = -0.80134 + 8.61223E-02T - 8.053232E-05T^2 + 6.3144787E-08T^3$
 $- 2.8327E-11T^4 + 5.325217E-15T^5$
 $\mu(110) = 7.78 \quad \mu(800) = 39.03 \quad \mu(1500) = 57.33$
~~std error est = 2.6E-02~~ ~~max error est = 0.06~~
 $T(\mu) = 22.84 + 9.70756\mu + 0.2197071\mu^2 + 1.0689525E-03\mu^3$
 $T(7.78) = 112 \quad T(39.03) = 800 \quad T(57.33) = 1503$
~~- std error est = 1.1~~ ~~max error est = 3.5~~
 NITROGEN N₂ 80-2200K
 $\mu(T) = 0.025465 + 7.5336535E-02T - 6.51566245E-05T^2 + 4.34945E-08T^3$
 $- 1.5622457E-11T^4 + 2.249666E-15T^5$
 $\mu(80) = 5.66 \quad \mu(1250) = 46.06 \quad \mu(2200) = 63.51$
~~std error est = 3.9E-02~~ ~~max error est = 0.11~~
 $T(\mu) = 23.03 + 9.279727\mu + 0.3237956\mu^2 + 1.14361184E-03\mu^3$
 $T(5.66) = 86 \quad T(46.06) = 1249 \quad T(63.51) = 2211$
~~- std error est = 1.5~~ ~~max error est = 11.0~~
 NITROGEN PEROXIDE NO₂ 300-450K
 $\mu(T) = 785.544557 - 8.749203T + 3.6259252E-02T^2 - 6.5336018E-05T^3$
 $+ 4.3577125E-08T^4$
 $\mu(300) = 13.02 \quad \mu(370) = 19.47 \quad \mu(450) = 24.09$
~~std error est = 9.4E-02~~ ~~max error est = 0.2~~
 $T(\mu) = 318.245 - 8.8194949\mu + 0.5945482\mu^2$
 $T(13.02) = 304 \quad T(19.47) = 372 \quad T(24.09) = 451$
~~- std error est = 2.7~~ ~~max error est = 6.0~~
 NITROUS OXIDE N₂O 180-1500K
 $\mu(T) = -1.4347 + 6.345024E-02T - 3.307219E-05T^2 + 1.3455025E-08T^3$
 $- 2.4171922E-12T^4$
 $\mu(180) = 8.99 \quad \mu(800) = 34.06 \quad \mu(1500) = 52.50$
~~std error est = 2.3E-02~~ ~~max error est = 0.04~~
 $T(\mu) = 30.57 + 15.037308\mu + 0.1758553\mu^2 + 1.3549377E-03\mu^3$
 $T(8.99) = 181 \quad T(34.06) = 800 \quad T(52.50) = 1501$
~~- std error est = 0.8~~ ~~max error est = 2.5~~

OCTAFLUOROCYCLOBUTANE C₄F₈ 270-440K

$$\mu(T) = -21.702187 + 0.29705496T - 1.1162856E-03T^2 + 2.126056E-06T^3 - 1.53345928E-09T^4$$

$$\mu(270) = 10.82 \quad \mu(350) = 13.67 \quad \mu(440) = 16.52$$

std error est = 1.2E-02 max error est = 0.15

$$T(\mu) = 51.767 + 13.95912177\mu + 0.574077\mu^2$$

$$T(10.82) = 270 \quad T(13.67) = 350 \quad T(16.52) = 439$$

$$- \text{std error est} = 0.6 \quad - \text{max error est} = 2.0$$

n-OCTANE C₈H₁₈ 300-650K

$$\mu(T) = 0.8324354 + 1.40045E-02T + 8.793765E-06T^2 - 6.8403E-09T^3$$

$$\mu(300) = 5.64 \quad \mu(450) = 8.29 \quad \mu(650) = 11.77$$

$$\text{std error est} = 2.1E-02 \quad \text{max error est} = 0.04$$

$$T(\mu) = -8.63 + 53.900825\mu + 0.167701848\mu^2$$

$$T(5.64) = 301 \quad T(8.29) = 450 \quad T(11.77) = 649$$

$$- \text{std error est} = 1.2 \quad - \text{max error est} = 3.5$$

OXYGEN O₂ 80-2000K

$$\mu(T) = -0.397863 + 8.7605894E-02T - 7.064124E-05T^2 + 4.6287E-08T^3 - 1.690435E-11T^4 + 2.534147E-15T^5$$

$$\mu(80) = 6.18 \quad \mu(1100) = 51.43 \quad \mu(2000) = 73.17$$

$$\text{std error est} = 3.1E-02 \quad \text{max error est} = 0.08$$

$$T(\mu) = 19.02 + 9.362836\mu + 0.185555\mu^2 + 7.899354E-04\mu^3$$

$$T(6.18) = 84 \quad T(51.43) = 1099 \quad T(73.17) = 2007$$

$$- \text{std error est} = 1.5 \quad - \text{max error est} = 7.0$$

n-PENTANE C₅H₁₂ 270-550K

$$\mu(T) = 0.2416119 + 2.307305E-02T - 1.52727E-06T^2$$

$$\mu(270) = 6.36 \quad \mu(400) = 9.23 \quad \mu(550) = 12.47$$

$$\text{std error est} = 8.2E-03 \quad \text{max error est} = 0.02$$

$$T(\mu) = -9.73 + 43.0470668\mu + 0.14747898\mu^2$$

$$T(6.36) = 270 \quad T(9.23) = 400 \quad T(12.47) = 550$$

$$- \text{std error est} = 0.4 \quad - \text{max error est} = 1.5$$

PROPANE C₃H₈ 270-600K

$$\mu(T) = -0.3543711 + 3.080096E-02T - 6.99723E-06T^2$$

$$\mu(270) = 7.45 \quad \mu(450) = 12.09 \quad \mu(600) = 15.61$$

$$\text{std error est} = 5.9E-03 \quad \text{max error est} = 0.01$$

PROPYLENE C₃H₆ 210-360K

$\mu(T) = -1.1116324 + 0.03663067T - 1.2184874E-05T^2$
 $\mu(210) = 6.04$ $\mu(300) = 8.78$ $\mu(360) = 10.50$
std error est = 4.4E-03 max error est = 0.01

210-360K

$T(\mu) = 36.1 + 25.971212587\mu + 0.4652205\mu^2$
 $T(6.04) = 210$ $T(8.78) = 300$ $T(10.50) = 360$
- std error est = 0.2 - - - - - max error est = 1.5

SULFUR DIOXIDE SO₂ 200-1250K

$\mu(T) = -1.141748 + 0.051281456T - 1.3886282E-05T^2 + 2.15266E-09T^3$
 $\mu(200) = 8.58$ $\mu(650) = 26.92$ $\mu(1250) = 45.47$
std error est = 3.7E-02 max error est = 0.08

200-1250K

$T(\mu) = 43.076 + 16.9625\mu + 0.20754597\mu^2$
 $T(8.58) = 204$ $T(26.92) = -50$ $T(45.47) = 1243$
- std error est = 2.2 - - - - - max error est = 9.0

TOLUENE C₇H₈ 330-550K

$\mu(T) = -2.2639265 + 3.8294535E-02T - 2.9042466E-05T^2 + 1.6824E-08T^3$
 $\mu(330) = 7.82$ $\mu(450) = 10.62$ $\mu(550) = 12.81$
std error est = 2E-02 max error est = 0.04

330-550K

$T(\mu) = 42.866 + 32.181384\mu + 0.579136617\mu^2$
 $T(7.82) = 330$ $T(10.62) = 450$ $T(12.81) = 550$
- std error est = 0.9 - - - - - max error est = 2.0

TRICHLOROFLUOROMETHANE CCl₃F 230-500K

(FREON-11)
 $\mu(T) = 4.6926597 + 5.81068E-03T + 6.427175E-05T^2 - 4.712105E-08T^3$
 $\mu(230) = 8.86$ $\mu(400) = 14.28$ $\mu(500) = 17.78$
std error est = 6E-03 max error est = 0.01

230-500K

$T(\mu) = -188.137 + 63.015166\mu - 2.19224063\mu^2 + 4.64365E-02\mu^3$
 $T(8.86) = 230$ $T(14.28) = 400$ $T(17.78) = 500$
- std error est = 0.3 - - - - - max error est = 1.5

TRICHLOROTRIFLUOROETHANE C₂Cl₃F₃ 230-400K

(FREON-113)
 $\mu(T) = 1.5959133 + 3.483849E-02T - 1.8833849E-05T^2$
 $\mu(230) = 8.61$ $\mu(350) = 11.48$ $\mu(400) = 12.52$
std error est = 4.9E-03 max error est = 0.01

230-400K

$T(\mu) = 23.38 + 10.69495544\mu + 1.547242767\mu^2$
 $T(8.61) = 230$ $T(11.48) = 350$ $T(12.52) = 400$
- std error est = 0.3 - - - - - max error est = 2.0

TRIFLUOROMETHANE CHF₃ 230-500K

$\mu(T) = -2.100796 + 6.3910783E-02T - 2.41926655E-05T^2$
 $\mu(230) = 11.32 \quad \mu(400) = 19.59 \quad \mu(500) = 23.81$
 std error est = 5.7E-03 max error est = 0.01

230-500K

$T(\mu) = 52.246 + 12.98628777\mu + 0.243660334\mu^2$
 $T(11.32) = 230 \quad T(19.59) = 400 \quad T(23.81) = 500$
 std error est = 0.2 max error est = 1.5

WATER H₂O 280-1000K

$\mu(T) = -3.07514683 + 4.069249E-02T + 5.20585924E-09T^2$
 $\mu(280) = 8.32 \quad \mu(650) = 23.38 \quad \mu(1000) = 37.62$
 std error est = 3.3E-03 max error est = 0.01

280-1000K

$T(\mu) = 75.57 + 24.574084\mu - 7.7339827E-05\mu^2$
 $T(8.32) = 280 \quad T(23.38) = 650 \quad T(37.62) = 1000$
 std error est = 0.08 max error est = 1.0

XENON Xe 120-1500K

$\mu(T) = 1.89178728 + 6.0506328E-02T + 8.1793523E-05T^2 - 2.051E-07T^3$
 $+ 2.0164963E-10T^4 - 9.5234E-14T^5 + 1.7662669E-17T^6$
 $\mu(120) = 10.02 \quad \mu(800) = 53.65 \quad \mu(1500) = 83.33$
 std error est = 4.2E-02 max error est = 0.07

120-1500K

$T(\mu) = 7.02702 + 11.3664655\mu + 0.0360854\mu^2 + 5.165008E-04\mu^3$
 $T(10.02) = 125 \quad T(53.65) = 800 \quad T(83.33) = 1504$
 std error est = 1.5 max error est = 4.5

APPENDIX D
TABLE D-I
SUMMARY OF CONTENTS

THE VIRIAL COEFFICIENTS
FOR GASEOUS ELEMENTS AND COMPOUNDS

NAME	FORMULA	APP D PAGE
Air (Dry, CO ₂ -free)	-	D-1
Argon	Ar	D-1
Carbon Dioxide	CO ₂	D-1
Deuterium	D ₂	D-1
Helium	He	D-2
Hydrogen	H ₂	D-2
Krypton	Kr	D-2
Methane	CH ₄	D-2
Neon	Ne	D-3
Nitrogen	N ₂	D-3
Oxygen	O ₂	D-3
Water Vapor	H ₂ O	D-4
'Heavy' Water Vapor	D ₂ O	D-4
Xenon	Xe	D-4

TABLE D-II Third Virial Coefficients D-5

APPENDIX D
FORMAT EXAMPLE

The equation/s is for gaseous Neon

The polynomial equation to calculate the SECOND virial coefficient [B(T)] in cm³/mol as a function of temperature (Kelvin)

Formula	Valid Temperature Range
NEON	<u>Ne</u>
	<u>80-200K</u>

$$B(T) = -108.0286 + 2.354366T - 2.011992E-02T^2 + 8.1876808E-05T^3 - 1.28414363E-07T^4$$

$$B(80) = -11.79 \quad B(140) = 2.57$$

std error est = 0.04

The standard (or average) error estimate over the temperature range noted is ±0.04 cm³/mol.

Using the polynomial presented, the calculated second virial coefficient at 200K is 7.60 cm³/mol.

Over the temperature range noted, the maximum error est is ±0.08 cm³/mol.

$$B(200) = 7.60$$

max error est = 0.08

FIGURE D-1

APPENDIX D

SECOND VIRIAL COEFFICIENTS
FOR GASEOUS ELEMENTS AND COMPOUNDS

AIR (Dry, CO ₂ -Free)	<u>100-150K</u>
B(T) = -1502.0253 + 31.45448274T - 0.279362289T ² + 1.1746791E-03T ³ - 1.91779611E-06T ⁴	
B(100) = -167.30 B(125) = -109.17 B(150) = -75.85 std error est = 4.3E-02 max error est = 0.1	
	<u>150-350K</u>
B(T) = -871.7496 + 14.673657T - 0.1155472T ² + 5.15056917E-04T ³ - 1.32633153E-06T ⁴ + 1.84350813E-09T ⁵ - 1.0723866E-12T ⁶	
B(150) = -75.88 B(250) = -19.77 B(350) = 0.42 std error est = 0.2 max error est = 0.6	
	<u>350-1400K</u>
B(T) = -113.0307 + 0.6191348T - 1.1961097E-03T ² + 1.2117027E-06T ³ - 6.19795E-10T ⁴ + 1.2599233E-13T ⁵	
B(350) = 0.53 B(800) = 24.75 B(1400) = 31.21 std error est = 0.092 max error est = 0.35	
ARGON Ar	<u>80-250K</u>
B(T) = -2602.5842 + 71.103308T - 0.8814188T ² + 5.9930164E-03T ³ - 2.3043749E-05T ⁴ + 4.704073E-08T ⁵ - 3.96383723E-11T ⁶	
std error est = 0.35 B(200) = -48.36 max error est = 0.9	
	<u>250-1500K</u>
B(T) = -195.60895 + 1.2604989T - 3.370398E-03T ² + 4.9626165E-06T ³ - 4.0932672E-09T ⁴ + 1.76812575E-12T ⁵ - 3.1081026E-16T ⁶	
B(250) = -27.93 B(700) = 15.23 B(1500) = 24.79 std error est = 0.16 max error est = 0.4	
CARBON DIOXIDE CO ₂	<u>250-1000K</u>
B(T) = -1495.9175 + 11.9968622T - 4.31032436E-02T ² + 8.501674E-05T ³ - 9.4651135E-08T ⁴ + 5.57671E-11T ⁵ - 1.3516095E-14T ⁶	
B(250) = -180.84 B(700) = -1.08 B(1000) = 14.31 std error est = 0.35 max error est = 1.0	
DEUTERIUM D ₂	<u>85-420K</u>
B(T) = -104.569 + 2.1780589T - 1.84434317E-02T ² + 8.7373826E-05T ³ - 2.36196123E-07T ⁴ + 3.3976588E-10T ⁵ - 2.0138934E-13T ⁶	
B(85) = -9.93 B(300) = 13.66 B(420) = 15.45 std error est = 0.7 max error est = 0.2	

HELIUM	He	<u>20-200K</u>
$B(T) = -34.55944 + 2.7175236T - 7.238207E-02T^2 + 1.0230434E-03T^3$		
- 7.80158414E-06T ⁴ + 3.01349506E-08T ⁵ - 4.60368796E-11T ⁶		
B(20) = -2.13	B(100) = 11.57	B(200) = 12.30
std error est = 0.14		max error est = 0.25
<u>275-1400K</u>		
$B(T) = 16.797 - 2.974167E-02T + 5.9985787E-05T^2 - 6.536E-08T^3$		
+ 3.4774704E-11T ⁴ - 7.17233967E-15T ⁵		
B(275) = 11.98	B(600) = 10.38	B(1400) = 8.40
std error est = 0.04		max error est = 0.09
<u>HYDROGEN H₂ 25-100K</u>		
$B(T) = -552.3468 + 37.9672515T - 1.2583684T^2 + 2.3661885E-02T^3$		
- 2.55707365E-04T ⁴ + 1.479355E-06T ⁵ - 3.547909E-09T ⁶		
B(25) = -106.23	B(50) = -33.48	B(100) = -2.52
std error est = 0.1		max error est = 0.25
<u>120-420K</u>		
$B(T) = -28.6784 + 0.2390086T + 1.6559E-03T^2 - 2.0165055E-05T^3$		
+ 7.74730172E-08T ⁴ - 1.3371575E-10T ⁵ + 8.80146735E-14T ⁶		
B(120) = 2.00	B(350) = 15.32	B(420) = 16.11
std error est = 0.04		max error est = 0.1
<u>KRYPTON Kr 125-200K</u>		
$B(T) = -3767.455 + 79.33045T - 0.7427849T^2 + 3.65588424E-03T^3$		
- 9.2488483E-06T ⁴ + 9.5193755E-09T ⁵		
B(125) = -284.18	B(160) = -178.36	B(200) = -117.39
std error est = 0.03		max error est = 0.1
<u>200-400K</u>		
$B(T) = -1195.697 + 14.577052T - 8.36262E-02T^2 + 2.714544E-04T^3$		
- 5.095532E-07T ⁴ + 5.16988543E-10T ⁵ - 2.19801246E-13T ⁶		
B(200) = -117.62	B(300) = -51.00	B(400) = -22.89
std error est = 0.04		max error est = 0.1
<u>400-1500K</u>		
$B(T) = -285.26 + 1.490866T - 3.3921494E-03T^2 + 4.3542916E-06T^3$		
- 3.1988343E-09T ⁴ + 1.253671E-12T ⁵ - 2.030971E-16T ⁶		
B(400) = -22.87	B(800) = 13.17	B(1500) = 27.00
std error est = 0.05		max error est = 0.1
<u>METHANE CH₄ 110-200K</u>		
$B(T) = -4564.8011 + 108.37155T - 1.1344657T^2 + 6.2125655E-03T^3$		
- 1.742442E-05T ⁴ + 1.9820625E-08T ⁵		
B(110) = -333.94	B(160) = -161.93	B(200) = -105.07
std error est = 0.04		max error est = 0.1

METHANE (continued) 200-400K

$$B(T) = -1161.958 + 14.527312T - 8.4895E-02T^2 + 2.7964493E-04T^3$$

$$- 5.300204E-07T^4 + 5.396463E-10T^5 - 2.28570436E-13T^6$$

$$B(200) = -105.11 \quad B(300) = -42.35 \quad B(400) = -15.73$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.07$$

400-1500K

$$B(T) = -263.0827 + 1.39774T - 3.15891435E-03T^2 + 4.03489206E-06T^3$$

$$- 2.954616E-09T^4 + 1.155816E-12T^5 - 1.87089616E-16T^6$$

$$B(400) = -15.75 \quad B(900) = 22.15 \quad B(1500) = 31.90$$

$$\text{std error est} = 0.06 \quad \text{max error est} = 0.15$$

NEON Ne 80-200K

$$B(T) = -108.0286 + 2.354366T - 2.011992E-02T^2 + 8.1876808E-05T^3$$

$$- 1.28414363E-07T^4$$

$$B(80) = -11.79 \quad B(140) = 2.57 \quad B(200) = 7.60$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.08$$

200-1000K

$$B(T) = -18.52 + 0.253489T - 8.9773E-04T^2 + 1.76985156E-06T^3$$

$$- 1.98866447E-09T^4 + 1.1902623E-12T^5 - 2.9438917E-16T^6$$

$$B(200) = 7.61 \quad B(600) = 13.77 \quad B(1000) = 14.30$$

$$\text{std error est} = 0.03 \quad \text{max error est} = 0.05$$

NITROGEN N₂ 100-150K

$$B(T) = -1934.0 + 49.775958T - 0.5771643T^2 + 3.5473302E-03T^3$$

$$- 1.12452359E-05T^4 + 1.45225962E-08T^5$$

$$B(100) = -159.85 \quad B(125) = -103.84 \quad B(150) = -71.41$$

$$\text{std error est} = 0.05 \quad \text{max error est} = 0.09$$

150-325K

$$B(T) = -1038.812 + 19.7330247T - 0.17557828T^2 + 8.834965E-04T^3$$

$$- 2.567272E-06T^4 + 4.0252916E-09T^5 - 2.6402379E-12T^6$$

$$B(150) = -71.65 \quad B(230) = -23.12 \quad B(325) = -0.36$$

$$\text{std error est} = 0.04 \quad \text{max error est} = 0.09$$

325-1400K

$$B(T) = -156.96 + 1.0434304T - 2.717715E-03T^2 + 3.9752575E-06T^3$$

$$- 3.3108834E-09T^4 + 1.462975E-12T^5 - 2.65735587E-16T^6$$

$$B(325) = -0.39 \quad B(800) = 27.37 \quad B(1400) = 33.50$$

$$\text{std error est} = 0.05 \quad \text{max error est} = 0.1$$

OXYGEN O₂ 100-200K

$$B(T) = -2793.674 + 78.48548T - 1.0166435T^2 + 7.34716756E-03T^3$$

$$- 3.052873E-05T^4 + 6.8392904E-08T^5 - 6.4137155E-11T^6$$

$$B(100) = -197.47 \quad B(150) = -90.79 \quad B(200) = -49.99$$

$$\text{std error est} = 0.035 \quad \text{max error est} = 0.08$$

OXYGEN (continued) 200-400K
B(T) = -499.657 + 5.4925876T - 2.7027447E-02T² + 7.1352086E-05T³
- 9.750388E-08T⁴ + 5.4294996E-11T⁵

B(200) = -50.05 B(300) = -15.69 B(400) = -0.60
std error est = 0.03 max error est = 0.05

400-1400K
B(T) = -165.1965 + 1.0063385T - 2.541077E-03T² + 3.630033E-06T³
- 2.9679937E-09T⁴ + 1.29213468E-12T⁵ - 2.318393E-16T⁶
B(400) = -0.61 B(900) = 21.01 B(1400) = 25.90
std error est = 0.02 max error est = 0.05

WATER VAPOR H₂O 430-720K

B(T) = -39636.088 + 319.317424T - 1.039708598T² + 1.69863388E-03T³
- 1.38836432E-06T⁴ + 4.53516028E-10T⁵
B(430) = -316.78 B(530) = -147.27 B(720) = -96.19
std error est = 0.6 max error est = 1.3

'HEAVY' WATER VAPOR D₂O 430-720K

B(T) = -40275.7499 + 324.5981063T - 1.057308467T² + 1.7280874E-03T³
- 1.41303458E-06T⁴ + 4.6177338E-10T⁵
B(430) = -320.24 B(550) = -133.22 B(720) = -56.19
std error est = 0.6 max error est = 1.5

XENON Xe 220-500K

B(T) = -2694.3436 + 32.305283T - 0.181532587T² + 5.744002E-04T³
- 1.04996174E-06T⁴ + 1.03791638E-09T⁵ - 4.30480244E-13T⁶
B(200) = -230.65 B(400) = -69.84 B(550) = -31.53
std error est = 0.05 max error est = 0.1

500-1500K
B(T) = -490.2594 + 2.20020277T - 4.4278794E-03T² + 5.059897E-06T³
- 3.3321925E-09T⁴ + 1.17879258E-12T⁵ - 1.735293E-16T⁶
B(500) = -38.78 B(1000) = 15.03 B(1500) = 30.09
std error est = 0.05 max error est = 0.1

TABLE D-II

THE THIRD VIRIAL COEFFICIENTS
OF GASEOUS ELEMENTS AND COMPOUNDS*

T, K	He	Ne	Ar	Kr	Xe	N ₂	O ₂	Air	H ₂	D ₂	H ₂ O	D ₂ O	CO ₂	CH ₄
25									14					
30									16					
35									14.3					
40									12.1					
45									10.7					
50									9.6					
55									8.9					
60	2.7	4							8.4					
70	2.5	4							7.4					
80	2.4	4	7						6.9					
90	2.3	4	9						6.4					
100	2.2	4	12						6.1	6				
110	2.1	3	16						5.9	5				
120	2.0	3	20						5.7	5				
130	1.9	3	23						5.5	5				
140	1.8	3	25					28	5.4	5				
150	1.7	3	23					26	5.3	5				
160	1.6	3	22			26	23	24	5.2	5				
180	1.5	3	20			21	20	21	5.0	5				
200	1.3	3	18			19	17	19	4.8	5				
220	1.2	3	16	33		17	15	18	4.6	5				
240	1.1	3	15	30		16	13	17	4.5	5				
260	1.1	3	13	28		15	12	16	4.4	5				
273	1.1	3	12	27	62	15	11	15	4.2	5		57	29	
280	1.0	3	12	26	59	15	11	15	4.1	5		56	28	
300	1.0	2	11	24	54	14	10	15	3.9	5		52	26	
320	1.0	2	11	23	50	14		14	3.6	5		49	25	
340	.9	2	10	21	46	14		14	3.4	5		45	24	
360	.8	2	9	20	41	13			3.2	5		42	22	
380	.8	2	9	19	36	13			3.0	4		38	19	
400	.7	2	9	18	34	13			2.9	4		36	17	
420	.7		9	18	32	12				3		32	16	
440			8	17	30	12							15	
460			8	16	28	12							14	
480			8	16	26	12							14	
500			7	15	24	12			-100	-150			14	
525			7	15	22				-53	-64			12	
550			7	14	20				-17	-20			12	
575			7	14	18				+2	0			11	
600			7	13					9	8			11	
650				13					12	12				
700				12					10	12				

*Units: 100 cm⁶/mol²

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